Frequency-independent voltage amplitude across a tunnel junction

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Radio-frequency (rf) scanning tunneling microscopy has recently been advanced to methods like single-atom spin resonance. Such methods require a frequency-independent rf voltage amplitude across the tunnel junction, which opposes the strong frequency dependence of the rf attenuation in a transmission line. A reliable calibration of the voltage amplitude across the tunnel junction is therefore crucial. Two calibration methods have been reported to date, both compensating for the frequency dependent rf attenuation (transfer function), which first has to be determined. In this work we present a method to achieve a frequency-independent rf voltage amplitude across the tunnel junction that avoids the detour of determining the transfer function, thus reducing the complexity of the calibration. We applied the method on our rf scanning tunneling microscope and show the results of the manual calibration. We also show the transfer function of our rf transmission line up to 5.6 GHz. Although this work has been conducted with a rf scanning tunneling microscope, the presented procedures should also apply to any other device that can deliver rf voltage to a tunnel junction.

I. INTRODUCTION

Scanning tunneling microscopy (STM) methods have been in constant development since its invention around 40 years ago.1, 2 One recently added method is radio-frequency scanning tunneling spectroscopy: voltage changes with radio-frequency (rf) are applied across the STM tunnel junction while the differential tunneling conductance $(\partial I/\partial V)$ is recorded.3 With this technique we have demonstrated excitation of electron and nuclear spin transitions in single molecules,4, 5 and have revealed mechanical eigenmodes of molecular resonators.6 A similar approach, well known as ESR-STM,7–12 is based on single-spin magnetoresistance detection and has recently enabled measurement of single-atom spin resonance.

One remaining technological challenge hampering the further development of rf STM is posed by the pronounced frequency dependence of the rf voltage amplitude across the tunnel junction ($V_{pk,jun}$). A variable $V_{pk,jun}$ may result in spurious measurement signals, which can easily be misinterpreted.13, 14 Therefore, a method to achieve constant $V_{pk,jun}$ independent of frequency, is imperative. Currently no method exists to measure $V_{pk,jun}$ directly.11 Two approaches for the determination of $V_{pk,jun}$ and its calibration to a constant value have been reported to date.13, 14 They rely on the comparison of differential tunneling conductance spectra and on the frequency dependent rf voltage attenuation (transfer function, see Appendix C) obtained using a linearization method for the nonlinear current-voltage characteristic of the tunnel junction. In this work, we present a method to achieve a constant $V_{pk,jun}$ independent of the comparison of conductance spectra, transfer function and linearization, which is based on a recursive algorithm.

II. RADIO-FREQUENCY SCANNING TUNNELING MICROSCOPE

We have conducted the experiments with a modified Createc low-temperature STM in ultra-high vacuum (UHV) conditions. The sample temperature is typically 8 K and the pressure below $5 \times 10^{-11}$ mbar. We have upgraded the STM with rf-rated components, similar to our previously reported setup.4, 6, 15 The schematic of the electronics is shown in Figure 1 and all components are listed in Appendix A. This setup enables rapid modulation of the voltage across the tunnel junction at high frequencies, achieving a bandwidth of up to $5.6 \text{GHz}$. The total voltage $V_{tot}$ is composed of two components, $V_{dc}$ and $V_{rf}$, which are superimposed:

$$V_{tot}(t) = V_{dc}(t) + V_{rf}(t).$$  (1)

Here $t$ is time, $V_{dc}$ is the slowly time-varying component ($\leq$ few kHz) and $V_{rf}$ is the fast time-varying component (rf voltage, MHz – GHz) with an amplitude of up to $\approx 100 \text{mV}$, limited by the attenuation in the transmission line (see Appendix C).

It is convenient to consider the electronic setup as three parts as shown in Figure 1. The dc and rf parts cover the electronics and cabling associated purely with the STM control and frequency modulation, respectively. In the mixed part, from the bias tees onward, the signals are transmitted through the same cables. Note that rf voltage is transmitted via cryo dc cables, which have an insertion loss (see Appendix C) of more than 60 dB/m at 2 GHz. Their length is $\approx 15$ cm each. Typical values of the insertion loss of all cables are given in Table II in Appendix A.

Although the insertion loss of the commercial electrical components is well specified, the determination of the to-
the determination of the tunneling current causes a broadening of the step as explained in the text. The dark green cross marks the value when the rf voltage amplitude is 20 mV and the light green cross when it is 30 mV. The shaded areas of the same colors illustrate the intervals that influence the corresponding $df/dv$-value at $V_{dc} = −85$ mV when rf voltage is applied.

One advantage of this method is that it is not necessary to know the exact functional relation between $P_{gen}$ and the $df/dv$-value. In particular, the relation does not need to be linearized nor fitted, unlike in the previously reported methods. A restriction is that the relation has to be bijective in the region of interest. This can be verified by recording $df/dv$ at a fixed $V_{dc}$ while sweeping $P_{gen}$. The nonlinearity causing the rectification has to be independent of the frequency and independent of the power of the rf voltage.

The success of the calibration can be quantified by determining the calibrated $V_{pk,jun}$ at each frequency and comparing it to the desired value. Figure 4 shows the result of a manual calibration. The desired value of 30 mV is met by the calibrated rf voltage amplitudes, which have a mean value of (30±2) mV. With future automation we expect to reduce the variance of the calibrated amplitudes. Additionally, improvements of the cabling and instrumentation will decrease the measurement error and raise the upper bandwidth limit to higher frequencies. The calibration for each frequency value takes about two minutes and the measurement of $V_{pk,jun}$ about ten minutes, including analysis and documentation. Once the automation is implemented, we expect both procedures to become significantly faster.

Based on our method to determine $V_{pk,jun}$, we also derived the transfer function of our setup as detailed in Appendix C.
FIG. 3. Exemplary time evolution of the $\frac{dI}{dV}$-value at constant $V_{dc}$ during calibration. In the first and last $\approx 4$ s, no rf voltage was applied. The times when the rf signal generator was switched on and off are marked with the annotations rf on and rf off, respectively. After the rf signal generator was switched on, $P_{\text{gen}}$ was adjusted until the target value was reached. The adjustment period is marked as manual adjustment and shaded in gray. The target $\frac{dI}{dV}$-value is drawn as a horizontal line. This example also highlights some potential issues with the manual procedure. Namely, the peak at $\approx 6$ s is caused by an unintentional fast variation of $P_{\text{gen}}$. The slower increase after $\approx 7$ s reflects the typical pace. Also, it is clear that some inaccuracy in the determination of the target value remains as the $\frac{dI}{dV}$ value between $\approx 20$ s and $\approx 30$ s is slightly too high. Automation of the procedure will improve this.

FIG. 4. Radio-frequency voltage amplitudes for 29 frequency values up to 5.6 GHz after manual calibration to the target value of 30 mV. The mean value of the calibrated amplitudes is $(30 \pm 2)$ mV, depicted by the dashed line. The frequency values were chosen by relevance to another experiment and are therefore not evenly distributed. With the future automation of the calibration we intend to reduce the variance of the amplitudes. Improvements of the cabling and instrumentation will reduce the measurement error and raise the upper bandwidth limit to higher frequencies.

IV. SUMMARY

Radio-frequency scanning tunneling spectroscopy is a powerful tool enabling, e.g., single-atom spin resonance. It requires a frequency-independent rf voltage amplitude across the tunnel junction, which is nontrivial. We have developed a new method to calibrate the rf voltage amplitude to a frequency-independent value. Unlike previously reported procedures, this method does not require the measurement of the transfer function of the rf transmission line, nor the linearization of the nonlinear current-voltage characteristic of the tunnel junction. First results show the successful application of our method: after calibration to the target value of 30 mV we measure a mean rf peak voltage across the tunnel junction of $(30 \pm 2)$ mV at 29 different frequencies up to 5.6 GHz. We also obtained the transfer function of the rf transmission line at these frequencies. Although this work has been achieved with a rf STM, we expect the described procedures to also apply to any other device that can deliver rf voltage to a tunnel junction.

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VI. DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.
Appendix A: Details of the electronic components

Tables I and II show details of the electronic components of the setup described in the main text in Section II.

TABLE I. Electronic components used in the STM transmission lines. The first two columns (nr, name) refer to Figure 1. The characteristic line impedance of components 1–6 and 9–13 is 50 Ω.

| nr | name description |
|----|------------------|
| 1  | rf GEN rf signal generator, Keysight N5173B |
| 2  | dc block Keysight N9398F |
| 3  | coax cable Mini-Circuits CBL-12FT-SMSM+ (12 ft) |
| 4  | bias tee Tektronix PSP5541A |
| 5  | feedthrough SMA on an UHV DN 16 CF flange |
| 6  | coax cable Lake Shore cryogenic cable SR (1.5 m) |
| 7  | cryo dc cable flexible cryogenic dc cable, < 0.15 m |
| 8  | cryo dc cable flexible cryogenic dc cable, < 0.15 m |
| 9  | coax cable Lake Shore cryogenic cable SR (1.5 m) |
| 10 | feedthrough SMA on an UHV DN 16 CF flange |
| 11 | bias tee Tektronix PSP5541A |
| 12 | high pass high pass filter, Mini-Circuits SHP-300+ |
| 13 | terminator Mini-Circuits, 50 Ω |

dc transmission line

I DSP STM electronic control box, Createc 6711 DSP (digital signal processor)
II coax cable bedea RG58 (5 m)
III low pass low pass filter, Mini-Circuits BLP-1.9+
IV amp FEMTO DLPCA-200
V coax cable low noise cable
V coax cable FEMTO CAB-LN1-BB (3 m)

TABLE II. Typical values of the insertion loss of the cables used in the rf transmission line. The numbers and names correspond to those in Table I and Figure 1. N/A means no data available for this entry.

| nr | name description | frequency (GHz) |
|----|------------------|-----------------|
| 3  | coax cable       | 0.50 0.73 1.00 1.37 2.00 5.00 6.00 |
| 6 & 9 | coax cable      | 4.43 N/A 6.27 N/A N/A 14.09 N/A |
| 7 & 8 | cryo dc cable   | 22.3 30.6 37.9 43.0 62.6 112.6 155.2 |

Appendix B: Determination of the rf voltage amplitude across the tunnel junction

The differential tunneling conductance \( \frac{dI}{dV} \) as a function of \( V_{dc} \) is measured with a lock-in amplifier. Typical values for the modulation rms voltage and frequency are a few mV and 773 Hz, respectively. We superimpose \( V_{rf} \) with frequencies up to several GHz. The resulting changes in \( \frac{dI}{dV} \) are too fast to be resolved by the lock-in amplifier, which outputs the time average of these changes.

If the time dependence of \( V_{rf} \) is known, a weight function \( u(\tau) \) for this averaging process can be calculated; the probability of \( V_{rf} \) having a value in the interval \( [V_{rf}, V_{rf} + dV_{rf}] \) is \( u(V_{rf}) \, dV_{rf} \). This probability is also equal to the time spent in this interval \( (dt) \) divided by the total time, \( T/(2f) \), that \( V_{rf} \) needs to run over all values between its extrema \(-V_{pk, jun}\) and \(+V_{pk, jun}\) once: \( u(V_{rf}) \, dV_{rf} = \frac{dt}{T/(2f)} \). (B1)

In our case, we use a sinusoidal modulation:

\[
V_{rf}(t) = V_{pk, jun} \sin(2\pi ft) \quad (B2)
\]

where \( V_{pk, jun} \) is the peak voltage amplitude across the junction and \( f \) the frequency. Thus, differentiating Equation (B2) and using the relation \( \cos(2\pi ft) = \sqrt{1 - \sin^2(2\pi ft)} \), Equation (B1) can be rewritten to give \( u(V_{rf}) \) explicitly,

\[
u(V_{rf}) = \frac{1}{\pi V_{pk, jun} \sqrt{1 - \left(\frac{V_{rf}}{V_{pk, jun}}\right)^2}}. \quad (B3)
\]

The weight function \( u(V_{rf}) \) has the shape of the probability density function of the arcsine distribution, \( \frac{1}{\pi \sqrt{1 - x^2}} \), see green line in Figure 6.

The time average of the differential tunneling conductance is obtained by convolution with \( u(V_{rf}) \),

\[
\frac{dI}{dV}(V_{dc}) = \int_{-V_{pk, jun}}^{+V_{pk, jun}} \frac{dI}{dV}(V_{dc} + V_{rf}) \, u(V_{rf}) \, dV_{rf}, \quad (B4)
\]

where \( \frac{dI}{dV}|_{rf\,on} \) and \( \frac{dI}{dV}|_{rf\,off} \) are the differential tunneling conductances with and without rf voltage applied, respectively. Figure 5 illustrates the convolution: the \( \frac{dI}{dV} \)-spectrum is averaged by the quickly oscillating \( V_{rf} \). The sinusoidal \( V_{rf} \) leads to a symmetric weight function. Therefore, the averaging affects the \( \frac{dI}{dV} \)-value only when the \( \frac{dI}{dV} \)-spectrum is nonlinear in the averaging range, \( V_{dc} \), which is the \( V_{dc} \)-interval \( [V_{dc} - V_{pk, jun}, V_{dc} + V_{pk, jun}] \). This well known effect of rectification at a nonlinearity has been described earlier in References 13, 14, 20–23.
In this work, we determine \( V_{\text{pk, jun}} \) using the characteristic step in the \( dI/dV \)-spectrum of Ag(111) as non-linearity. Similar procedures have been successfully applied to spectroscopic features of, e.g., a Co atom on MgO/Ag(001).\(^{14}\) The step corresponds to the onset of the electronic surface state near \(-70\) mV.\(^{24}\) When measured with \( V_{\text{rf}} \) applied, this step is broadened, as shown in Figure 5. Based on Equation B4 we determine \( V_{\text{pk, jun}} \) by a series of \( dI/dV \)-measurements and a computer simulation. We record the \( dI/dV \)-spectrum of Ag(111) without \( V_{\text{rf}} \) and the \( dI/dV \)-spectrum with \( V_{\text{rf}} \) switched on (the latter is herein denoted by \( r f dI/dV \)-spectrum). The \( dI/dV \)-spectra are averages of five consecutive measurements at the same point on the silver surface. They are recorded typically within one minute to minimize the effects of slow changes at the tunnel junction such as thermal drift or a tip apex rearrangement.

Since \( u(V_{\text{rf}}) \) is a function of \( V_{\text{pk, jun}} \), see Equation B3, \( V_{\text{pk, jun}} \) can be used as an independent variable (simulation parameter) in the computer simulation. For a set of test values of \( V_{\text{pk, jun}} \) the \( dI/dV \)-spectrum without \( V_{\text{rf}} \) is convolved with \( u(V_{\text{rf}}) \), yielding simulated rf \( dI/dV \)-spectra. These, we compare to the measured rf \( dI/dV \)-spectrum by a least-squares analysis. The simulated spectrum with the lowest sum of squared residuals yields our best guess for the value of \( V_{\text{pk, jun}} \). An additional analysis of the residuals is used to identify unreliable simulation results due to the aforementioned slow changes at the tunnel junction that can occur during measurements. An example of the \( dI/dV \)-spectra used for the determination of \( V_{\text{pk, jun}} \) at one single frequency is shown in Figure 5. The simulated rf \( dI/dV \)-spectrum agrees very well with the measured rf \( dI/dV \)-spectrum.

**Appendix C: Transfer function**

The electric power loss between two points 1 and 2 along a rf transmission line is frequency-dependent.\(^{25}\) We describe the power loss with the frequency-dependent transfer function \( T_p \). It is defined by

\[
T_p := 10 \log_{10} \left( \frac{P_2}{P_1} \right) \tag{C1}
\]

where \( P_1 \) and \( P_2 \) are the powers in watts at point 1 and point 2, respectively. The subscript \( r f \) signifies that this definition is based on the ratio of powers. \( T_p \) is a level quantity,\(^{23}\) i.e., it compares two values. The unit of \( T_p \) is the decibel (dB). Note that the insertion loss\(^{25}\) of the transmission line between the points 1 and 2 is \(-T_p\).

It is common to express the power (\( P \)) of a rf voltage signal compared to the fixed reference value of \( 1 \) mW. This defines the power level (dBm) as

\[
dbm P := 10 \log_{10} \left( \frac{P}{0.001} \right). \tag{C2}
\]

Its unit is the dBm. Note that \( dbm P \) is a level quantity and it is therefore intrinsically different from the power quantity \( P \). Expressing \( P \) in terms of \( dbm P \), Equation C1 becomes

\[
T_p = dbm P_2 - dbm P_1 \tag{C3}
\]

where \( dbm P_1 \) and \( dbm P_2 \) are the power levels at point 1 and point 2, respectively.\(^{26}\)

In order to characterize the whole transmission line, here the output of the rf signal generator is chosen as point 1 and the sample surface as point 2, giving

\[
T_p = dbm P_{\text{sam}} - dbm P_{\text{gen}} \tag{C4}
\]

where \( dbm P_{\text{sam}} \) and \( dbm P_{\text{gen}} \) are the corresponding power levels.

In practice, it is convenient to express the transfer function in terms of a ratio of voltages rather than powers. The conversion from power to voltage requires knowledge about the impedance.\(^{25}\) The mean power dissipated by an ohmic impedance (\( R \)) in a rf circuit is

\[
P = \frac{V_{\text{rms}}^2}{R} \tag{C5}
\]

where \( V_{\text{rms}} \) is the root mean square voltage. For sinusoidal modulation, it is related to the peak voltage (\( V_{\text{pk}} \)) by

\[
V_{\text{pk}} = V_{\text{rms}} \sqrt{2}. \tag{C6}
\]
The conversion between \(^{\text{dBm}} P\) and \(V_{\text{pk}}\) can be done using Equations C2, C5 and C6, giving

\[
V_{\text{pk}} = \sqrt{\frac{2R}{1000}} 10^{\left(\frac{^{\text{dBm}} P}{10}\right)} \ .
\]  

(C7)

When using the line impedance of our components of 50 Ω, Equation C7 simplifies to

\[
V_{\text{pk}} = \sqrt{10^{\left(\frac{^{\text{dBm}} P}{10}\right)}} \ .
\]  

(C8)

Equation C8 is valid for \(^{\text{dBm}} P\) in dBm and \(V_{\text{pk}}\) in V.

Using Equation C5, Equation C1 can be transformed to

\[
T_p = 20 \log_{10} \left(\frac{V_2}{V_1}\right) - 10 \log_{10} \left(\frac{R_2}{R_1}\right)
\]  

(C9)

where \(V_1\) and \(V_2\) are the voltages at point 1 and point 2, respectively, and \(R_1\) and \(R_2\) the corresponding line impedances. \(V_1\) and \(V_2\) have to be the same entity, e.g., \(V_{\text{rms}}\) or \(V_{\text{pk}}\). If the impedances are the same, the second term vanishes. Considering the abovementioned locations (point 1: output of the rf signal generator, point 2: sample surface), this may not be the case in general. Therefore we define a separate transfer function \(T\), which is independent of the impedances (cf. Reference 16),

\[
T := 20 \log_{10} \left(\frac{V_{\text{pk, jun}}}{V_1}\right) \ .
\]  

(C10)

Here, \(V_2\) corresponds to \(V_{\text{pk, jun}}\) and \(V_1\) to the peak amplitude of the voltage of the rf signal generator output \((V_{\text{pk, gen}})\). Hence,

\[
T := 20 \log_{10} \left(\frac{V_{\text{pk, jun}}}{\text{pk, gen}}\right) \ .
\]  

(C11)

With the measured rf voltage amplitudes across the tunnel junction, the corresponding \(P_{\text{gen}}\) and Equation C8, we calculated the transfer function \(T\) according to Equation C11. \(T\) as a function of the frequency is shown in Figure 6. Its value varies from \((-3\pm 1)\) dB at 0.2 GHz to \((-46\pm 1)\) dB at 5.4 GHz. Below 1 GHz, it stays above \(-20\) dB. Between 1 and 5 GHz it varies between \(-20\) and \(-40\) dB. Between 5 and 6 GHz it drops below \(-40\) dB.

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26. When subtracting two level quantities with the unit dBm, the result is a level quantity in dB. Substitution of Definition C2 into Equation C3 and a short calculation make this clear.