Lock-in Amplifier Operation for dI/dV Mapping via Scanning Tunneling Microscopy

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1 Overview

Usage of lock-in amplifier theory and amplifiers are common in the experimental science as a measurement technique in noisy environments. Basically, a reference signal is introduced to an experimental parameter and a filter is used to extract the signal with same modulation frequency.

In the case of Scanning Tunneling Microscopy (STM) measurements, this operation is used as a way to map the differential conductivity (dI/dV) of the specimen at a constant energy. In this work we discuss the principal theory behind this operation. In the figure 1, the general schematics of the experimental setup can be seen.

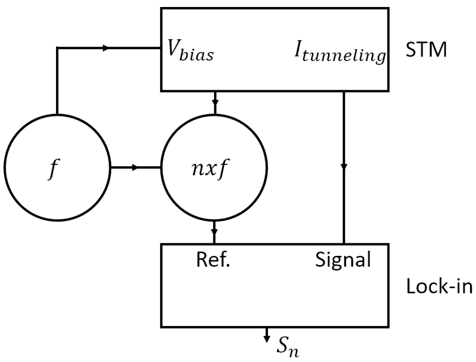

Figure 1: Depiction of the experimental setup with STM and lock-in detection. A wave generator is used to oscillate the V_{bias} of the system and this cause an oscillation of the $I_{tunneling}$ between the surface and tip. The lock-in amplifier multiplies this signal with the reference signal coming from the wave generator to detect the quantity of signal at the exact modulation frequency.

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2 Analysis

In this model we assume our wave generator produce perfect sine wave with the value of $U_0 sin(2\pi f t)$.

$$U(t) = V_{bias} + U_0 sin(2\pi f t) \tag{1}$$

This signal as equation 1 suggests, added to V_{bias} . Also it runs through the lock-in amplifier as a reference signal. It should be noted that the frequency can contain higher harmonics of the f. The nxf indicates this. In STM, the tunneling current that caused by the quantum tunneling phenomena is a function of the bias voltage. And with the addition of the driving signal this V_{bias}, it is now become a function time,

$$I_{tunneling} = I_{tunneling}(V_{bias}) = I_{tunneling}(V_{bias}(t)) \tag{2}$$

It should also be noted that, the signal that run through the lock-in amplifier is not the $I_{tunneling}$ but the voltage value that converted from $I_{tunneling}$ in the STM system with an I-V converter.

After two signals fed to the lock-in amplifier, the operation performed. The operation is basically multiplying the two signal ad then integrated over a longer time than the periodicity of the signals. The lock-in operation is;

$$S_n = \frac{1}{T} \int_o^T sin(2\pi f t + \delta\phi) I_{tunneling}(t) dt \tag{3}$$

where $T = \frac{m}{f}$, while m is an integer $\gg 1$, indicates relatively long time. And $\delta\phi$ is phase shift, possibly from different signal path of variables. In order to perform this operation we need the Taylor expansion of the $I_{tunneling}$. From Taylor expansion $I_{tunneling}(V_{bias})$ around $U(t=0) = V_{bias}$;

$$\begin{aligned} I_t(V) &= \sum_{\alpha=0}^{\infty} \frac{1}{\alpha!} I^{(\alpha)} (V - V_0)^{\alpha} \\ I^{(\alpha)} &= \left(\left(\frac{\partial}{\partial V} \right)^{\alpha} I_t \right)_{V=V_0} \end{aligned} \tag{4}$$

Also we expand the bias voltage as a function of time into its Fourier series to be able to multiply it with Taylor expansion of the tunneling current to check orthogonality.

$$V(t) = \sum_{\mu=0}^{\infty} V_{\mu} sin(2\pi f \mu t + \delta\phi_{\mu}) \tag{5}$$

In order to avoid further complications, we will use abbreviation instead of the sine values;

$$s_{\mu} = sin(2\pi f \mu t + \delta\phi_{\mu}) \tag{6}$$

Then, the Fourier series of the bias voltage is;

$$V(t) = \sum_{\mu=0}^{\infty} V_{\mu} s_{\mu} \tag{7}$$

From Taylor expansion;

$$I(t) = \frac{1}{0!} I (V - V_0)^0 + \frac{1}{1!} \left(\frac{\partial I}{\partial V} \right)_{V_0} (V - V_0)^1 + \frac{1}{2!} \left(\frac{\partial^2 I}{\partial V^2} \right)_{V_0} (V - V_0)^2 + \dots \tag{8}$$

And using only the first two harmonics;

$$V(t) = V_0 + V_1 s_1 \tag{9}$$

The reason that just $\mu = 0.1$ cases were used is because we add just one extra signal to our bias voltage. Even this is not the case the physical parameters mostly have negligible magnitude at higher harmonics.

If we explicitly write the Taylor expansion of current by taking into account the voltage;

$$\begin{aligned} I(t) = (I)_{V_0} + \left(\frac{\partial I}{\partial V}\right)_{V_0} (V_0 + V_1 s_1 - V_0) + \frac{1}{2}\left(\frac{\partial^2 I}{\partial V^2}\right)_{V_0} (V_0 + V_1 s_1 - V_0)^2 \\ = (I)_0 + \left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 s_1 + \frac{1}{2}\left(\frac{\partial^2 I}{\partial V^2}\right)_{V_0} {V_1}^2 {s_1}^2 \end{aligned} \tag{10}$$

From equation 3 and 10;

$$\begin{aligned} S_n &= \frac{1}{T}\int_0^T s_1 \left[I_0 + \left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 s_1 + \frac{1}{2}\left(\frac{\partial^2 I}{\partial V^2}\right)_{V_0} {V_1}^2 {s_1}^2 \right] \partial t \\ &= \frac{1}{T}\int_0^T \left[I_0 s_1 + \left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 {s_1}^2 + \frac{1}{2}\left(\frac{\partial^2 I}{\partial V^2}\right)_{V_0} {V_1}^2 {s_1}^3 \right] \partial t \end{aligned} \tag{11}$$

We are going to introduce the trigonometric identity in order to evaluate the sinusoidal multiplications;

$$sin(x)sin(y) = \frac{1}{2}\left(sin\left(x - y + \frac{\pi}{2}\right) + sin\left(x + y + \frac{\pi}{2}\right)\right) \tag{12}$$

Just consider first two term;

$$S_n = \frac{1}{T}\int_0^T \left[I_0 sin\left(2\pi f t + \delta\phi_1\right) + \frac{1}{2}\left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 \left(sin\left(\frac{\pi}{2}\right) + sin\left(4\pi f t + 2\delta\phi_1 + \frac{\pi}{2}\right)\right)\right] \partial t \tag{13}$$

First part of the integral;

$$\int_0^T I_0 sin(2\pi f t + \delta\phi_1)\partial t = \frac{I_0}{2\pi f}\left(cos(\delta\phi_1) - cos(2\pi f T + \delta\phi_1)\right) \tag{14}$$

And the second part;

$$\begin{aligned} \frac{1}{2}\int_0^T \left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 \left(sin\left(\frac{\pi}{2}\right) + sin\left(4\pi f t + 2\delta\phi_1 + \frac{\pi}{2}\right)\right) \partial t \\ = \frac{1}{2}\left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 T + \frac{1}{2}\left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 \frac{1}{2\pi f}\left[cos\left(2\delta\phi_1 + \frac{\pi}{2}\right) - cos\left(4\pi f t + 2\delta\phi_1 + \frac{\pi}{2}\right)\right] \end{aligned} \tag{15}$$

Thus;

$$\begin{aligned} S_n = \frac{I_0}{2\pi f T}\left[cos(\delta\phi_1) - cos(2\pi f T + \delta\phi_1)\right] + \frac{1}{2}\left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 \\ + \frac{1}{2}\left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 \frac{1}{2\pi f T}\left[cos\left(2\delta\phi_1 + \frac{\pi}{2}\right) - cos\left(4\pi f T + 2\delta\phi_1 + \frac{\pi}{2}\right)\right] \end{aligned} \tag{16}$$

If initial phase difference is equal to zero ($\delta\phi_1 = 0$), and we know $T = \frac{m}{f}$ while m is an integer $\gg 1$;

$$
\begin{aligned}
S_n = \frac{I_0}{2\pi f T}\left[1 - cos(2\pi m)\right] + \frac{1}{2}\left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 \\
+\frac{1}{2}\left(\frac{\partial I}{\partial V}\right)_{V_0} V_1 \frac{1}{2\pi f T}\left[cos\left(\frac{\pi}{2}\right) - cos\left(4\pi m + \frac{\pi}{2}\right)\right]
\end{aligned}
\tag{17}
$$

$$
S_n = \frac{V_1}{2}\left(\frac{\partial I}{\partial V}\right)_{V_0}\left(1 - \frac{1}{wT}\right) \tag{18}
$$

The expression $\left(\frac{\partial I}{\partial V}\right)_{V_0}$ is crucial in here, which is the differential conductivity at constant bias voltage which concludes our efforts.

3 Acknowledgements

This work is written under the guidance of the Assoc. Prof. Oğuzhan Gürlü. We used Ralf Vogelgesang's "Lock-In Amplifier Theory" whitepaper [1] extensively as the main source of this work. We also would like to thank our lab mates at NanoBEEs of Istanbul Technical University for the patience and attention, when we lecture this work.

References

[1] Ralf Vogelgesang. Lock-In Amplifier Theory. `http://www.nanooptics.ch/images/stories/personalNotes/LockIn.pdf`, 11/03/2018.