Vibration Mitigation for Atomic-Resolution Imaging

Albert Chien
Harvard John A. Paulson School of Engineering and Applied Sciences
Harvard University

Faculty Advisor
Jennifer E. Hoffman

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I would like to dedicate my thesis to my family and friends for their love and support throughout my time in college.
Abstract

Scanning tunneling microscopes (STM) are sensitive devices that can measure atoms and their electronic structures. To make these measurements, vibrations from the environment must be isolated from the microscope. Present passive vibration isolation systems reduce vibrations to the picometer level, yet certain electronic structures remain difficult to resolve. This thesis presents a post-processing solution which can be used in conjunction with passive systems to further reduce vibration noise in measurements. The solution consists of two parts: calibration and cancellation. The calibration process characterizes how vibrations propagate from a geophone to the microscope. The cancellation process records vibrations on the same geophone as researchers collect data on the STM. Then, the data is processed to remove vibration noise using the geophone signal. The solution achieved noise reduction under both standard microscope operating conditions and transient noisy conditions. A reduction in noise relatively strengthens the signal, reduces scanning time, enlarges the scanning area, and improves the resolution of data on the STM. Since the solution only requires a geophone and a suitable data acquisition device, the post-processing method could be implemented broadly across various vibration-sensitive equipment. Potential applications of this method could range from desktop scanning electron microscopes to LIGO observatories.
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Chapter 1

Introduction

1.1 Background

A scanning tunneling microscope (STM) is an atomic resolution microscope that
scans a sharp tip across a sample surface and examines the electronic properties by
quantum tunneling. Quantum tunneling occurs between the tip and sample, usually
separated by 4-7 angstroms, to allow electrons to tunnel from the sample surface to
the microscope tip.[1] The tunneling current is exponentially dependent on the tip-

sample distances. A STM is mainly used to collect two types of data: topographic
data and spectroscopic data (see Figure 1.2). To collect topographic data, the tip
scans across a sample at a constant voltage and a PI controller holds the current
constant by changing the Z position of the tip. To collect spectroscopic data, the STM fixes the spatial location of the tip, turns off the feedback loop, and measures
the tunneling current while sweeping the voltage. The change in tunneling current
with voltage is proportional to the density of states in a material, a key quantity
sought by researchers.

Vibrations cause noise in measurements and the signal-to-noise of a STM lim-
1.1 Background

Figure 1.1: Schematic view of a scanning tunneling microscope. When a sharp metallic tip is brought to within a few angstroms of a conducting sample, a current is induced by quantum tunneling. A STM uses a feedback loop to maintain a stable current so that it remains at a fixed height above the sample, allowing it to image atomic-scale features as the tip is moved across the sample. [2]

Figure 1.2: STM collects topographic and spectroscopic information. Left: In topographic scans, it measures surface morphology and can identify single-atom defects, such as this missing Sb atom in CeSb. Right: In spectroscopic measurements, it measures density of electronic states from $dI/dV$ curves, which have peaks and troughs of interest to researchers.
its the quality of data a researcher can obtain from the microscope. For example, the candidate strongly correlated topological insulator SmB$_6$–a material actively researched in the Hoffman lab–has a small Fermi surface pocket around the $\bar{\Gamma}$ point with radius $k(E_F) \sim 0.09\,\text{Å}^{-1}$, which decreases in size as energy (or bias) is lowered, eventually vanishing at the Dirac point, where $k(E_D) \sim 0\,\text{Å}^{-1}$.[3] In a STM spectroscopic measurement, this feature generates standing waves around atomic defects, called quasiparticle interference, whose wavelength is governed by the $k(E)$ dispersion. The ability to resolve these waves depends on the size of the real space image. For typical measurement conditions, the Hoffman Lab STM can reliably capture a 60 nm by 60 nm square image, corresponding to a maximum resolution of $\sim 0.002\,\text{Å}^{-1}$, before depletion of liquid Helium in the dewar destabilizes the temperature of the microscope (about 3-4 days). The acquisition time is proportional to the image size squared, with the proportionality constant related to the signal-to-noise ratio of the microscope; a microscope with lower signal-to-noise must spend more time at each pixel. A significant reduction of noise by post-processing vibration cancellation would enable faster acquisition speeds, larger real-space images, and higher k-space resolution. A 80% noise reduction would increase the image size to 130 nm by 130 nm, corresponding to a maximum resolution of $0.0008\,\text{Å}^{-1}$, and improve the labs ability to resolve small features like those close to the Dirac node in SmB$_6$.

**1.2 Problem Definition**

Measurements on a STM are on the scale of picometers and picoamperes, and are exponentially dependent on the distance between the tip and sample surface. Mechanical vibrations that reach the STM on the order of picometers become problematic for measurements.[4] Modern STM labs use multiple passive methods to reduce ambient noises. These ambient noises include mechanical vibrations, acoustic noise, and
electromagnetic waves. For example, state-of-the-art microscopes employ large pneumatic cylinders and inertial blocks that reduce external vibrations from the micron scale to the picometer scale at the STM tip.[5] These vibration isolation stages increase the signal-to-noise ratio and allow for a clear picture of the atomic structure of a sample. Yet, even the best microscopes still experience ambient noise in the range of picometers at certain frequencies and experience difficulty resolving electronic signatures such as the density of states of samples; vibrational noise is a fundamental limit in STM studies of complex materials and the characteristics of materials. Vibrations are especially problematic below 120 Hz, where electrical devices and the building in which the microscope is housed generate a lot of noise. Specifically, people walking in the building cause vibrations at \( \sim 3 \text{ Hz} \), the building floors have diaphragm modes at \( \sim 20 \text{Hz} \), and typical cryopumps operate at \( \sim 57 \text{Hz} \), with higher harmonic frequencies detected by the STM. These vibrations also couple with and excite the natural resonance frequencies of the STM, as shown in Figure 1.3. Therefore, this project aims to reduce mechanical noise and improve the signal-to-noise ratio at the STM tip beyond the present levels attained with passive isolation systems.

1.3 State of the Art

There is a multitude of previous work that has theoretically and experimentally characterized the ambient noise in STMs. There have been multiple papers published on the vibration isolation analysis of STMs since the invention of STM.[7] For example, Olivia et al. modelled an STM as a three-stage mass-spring damper system and characterized its frequency response across various masses, spring constants, and damping constants.[4] Iwaya et al. also extensively analyzed the vibration sources for a STM setup similar to that in the Hoffman Lab. They constructed a passive and active noise isolation system employing off-the-shelf parts from Tokkyoikiki Cor-
1.3 State of the Art

Figure 1.3: Frequency spectrum of ambient noise as detected on a STM tip in Hoffman Lab. Even a passively isolated STM, such as this one in the Hoffman lab, measures ambient noise of around 1 pm root mean squared (RMS) integrated over a 1 kHz bandwidth. The frequency spectrum reveals the sources of noise based on the resonant frequency. The ambient noise can overwhelm small surface features of interest (less than 2 pm). [5] [6]
1.3 State of the Art

(a) A twin-tip setup with one tip detecting vibrations to cancel noise in the other tip. The measured vibrations from one tip is filtered and fed-forward to cancel mechanical noise from the other tip. This implementation requires custom hardware and cannot be retroactively applied to current microscopes.

(b) Active noise cancellation system using an accelerometer and an ANITA processor. A similar concept to the twin-tip setup, but with an accelerometer close to the tip to detect vibrations. This scheme requires a custom processor to actively cancel vibrations in real time.

Figure 1.4: Active noise cancellation methods addressing ambient noise in a STM.

Figure 1.5: Vibrations attenuate and phase-shift while propagating from the geophone to the tip. A geophone attached to the top of the microscope (green) measures external vibrations as they enter the system. The vibrations (yellow arrow) are attenuated and phase-shifted as they travel to the microscope tip (orange).
algorithm processes the signal from an accelerometer and preemptively moves the tip to suppress vibrational noise (see Figure 1.4b). The group tested the system by driving vibrational noise with a mass-loaded DC motor and showed promising results for eliminating noise at the driven frequency. This being said, their method performs best for isolated single frequencies that provide a coherent source of noise and may be limited in reducing the typical incoherent ambient noise encountered in the lab. Furthermore, the two aforementioned methods actively cancel noise from measurements, which makes delineating the effects of a signal and the effects of the active noise cancellation a difficult task. In another approach, Bryce Primavera, a former Hoffman lab student, developed a post-processing method which preserves the original measurements. He pioneered a method of reducing picometer vibrations through post processing of the measured signal. His method employed a geophone attached to the base of the microscope arm and recorded the external noise just before it reaches the tip. The mechanical structure between the geophone and tip uniquely attenuates or amplifies and phase-shifts each frequency. A calibration procedure measures this attenuation and phase-shift, which yields a transfer function in the frequency domain. In subsequent measurements, detected vibrations from the geophone can be coupled with the transfer function to estimate their impact at the tip. This estimated noise is subtracted from the measured STM signal in a post-processing step. The simple method achieved a 48% attenuation of root-mean-squared (RMS) noise from 683 fm to 353 fm across a 0-100 Hz bandwidth.[5] However, his work focused on cancelling topographic noise and the post-processing method is detached from the present workflow of researchers. This project attempts to extend beyond the achievements of his work by applying the post-processing method to topographic scan images, incorporating the work within the present data collection workflow, and extending the scheme to cancel spectroscopic noise.
1.4 Targeted Users

As this project works closely with the Hoffman Lab, the main users of the solution will be researchers within the lab who collect and analyze topographic and spectroscopic STM data. Reducing mechanical noise in the system will improve the quality of data from the STM and further their mission to understand and control the nanoscale electronic and magnetic properties of exotic materials. However, the solution could also have an impact on all users of STMs. There are different sizes of STMs available to users; the difference between STMs mainly lie within a trade-off between the physical size and vibration isolation capabilities of the STM. Commercial vendors such as AFM Workshop and Nanosurf offer desktop STMs that are compact but noisy.[11][12] On the custom-built end, there are many research labs that have precise STMs occupying entire rooms in the basement of buildings. Yet, a noise cancellation algorithm could be applied to improve the performance of both categories of STMs. In particular, the compact size of a post-processing vibration mitigation technique, typically involving a geophone coupled to the STMs data collection system, may be applicable to commercial STMs and reduce noise below the picometer scale. The additional noise cancellation would augment the mechanical noise cancellation of custom-built STMs and improve researchers ability to detect weak signals. Hence, the post-processing vibration mitigation scheme would be an attractive offering to users of all STMs.

1.5 Design Specifications

To evaluate the success of the solution, a set of technical specifications based on the problem outlined in Section 1.2 was defined and can be found in Table 1.1 below. The specifications cover three areas of the solution: the level of noise attenuation achieved,
1.5 Design Specifications

the operating range of the noise attenuation, and the implementation-related characteristics of the solution.

Since noise is analogous to deviations in a measured signal from the true signal, a zero-centered signal’s root mean squared (RMS) value can quantify the noise within a measurement. Then, the percent reduction in RMS value of a signal before and after processing can indicate the level of noise attenuated. Previously, Primavera demonstrated a 48% reduction in ambient topographic noise and this project aims to increase the level of noise reduction to $> 80\%$. The increased signal-to-noise ratio would expand the spectroscopic map size from the present 60 nm by 60 nm to a possible 90 by 90 nm, corresponding to a maximum resolution of 0.0011 Å$^{-1}$.

The operating range of the noise attenuation must cover possible operating conditions for the STM. On one end of the range under the best possible operating conditions, ambient conditions have little to no vibrational noise in the STM and all passive isolation systems (pneumatic isolators, liquid Helium temperatures, vacuum conditions) are active. On the other end of the range under poor operating conditions, there is a driven noise source detectable on the STM with all passive isolation systems engaged. This mirrors instances when cryopumps in the vicinity of the Hoffman Lab STMs generate vibrational noise around 57 Hz. Combinations of the different operating conditions and the different data types (topographic and spectroscopic) lead to the first four technical specifications for the desired noise reduction levels. A noise attenuation bandwidth of 0-300 Hz is desirable as this bandwidth encompasses most detectable mechanical noise sources and their higher harmonics within a building.

A successful implementation of the post-processing vibration mitigation scheme must be usable for researchers on a continual basis. This requires an easy-to-use control interface and a relatively fast processing time to minimize disruptions to a researcher’s workflow. The main programming languages used in the Hoffman Labs and in many other STM labs are LabVIEW and Python. As such, the implementation
must be executable in those languages for easy incorporation within present workflows. Additionally, raw topographic and spectroscopic data can contain millions of data samples. The algorithm must either concurrently or near-simultaneously process data as the scanning proceeds to minimize the additional time for processing and the disk storage usage for sample data.

**Table 1.1: Technical Specifications**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Functional Requirement</th>
<th>Achieved Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient Topographic RMS Noise Reduction</td>
<td>&gt; 80%</td>
<td>20.9% ± 3.6%</td>
</tr>
<tr>
<td>Driven Topographic RMS Noise Reduction</td>
<td>&gt; 80%</td>
<td>81.5% ± 6.4%</td>
</tr>
<tr>
<td>Ambient Spectroscopic RMS Noise Reduction</td>
<td>&gt; 80%</td>
<td>-</td>
</tr>
<tr>
<td>Driven Spectroscopic RMS Noise Reduction</td>
<td>&gt; 80%</td>
<td>65.4% ± 8.7%</td>
</tr>
<tr>
<td>Noise Attenuation Bandwidth</td>
<td>0 – 300 Hz</td>
<td>0 – 300 Hz</td>
</tr>
<tr>
<td>Usability</td>
<td>Executable in LabVIEW or Python</td>
<td>LabVIEW UI and Python back-end</td>
</tr>
<tr>
<td>Speed</td>
<td>Simultaneous to Data Collection</td>
<td>Within 5 minutes of scan completion</td>
</tr>
</tbody>
</table>
Chapter 2

System Design

Summary

To satisfy design specifications outlined in Section 1.5, the designed solution includes careful considerations on both the theoretical and implementation level. Section 2.1 Theoretical Background gives an outline of the noise cancellation scheme for both topographic and spectroscopic data. Section 2.2 System Implementation highlights the overall interactions within the system, as well as a deeper inspection of critical components of the system. The built system as described is then tested and analyzed in subsequent chapters of this report.

2.1 Theoretical Background

2.1.1 Topographic Cancellation

Due to the placement of the geophone outside the vacuum can and some distance from the tip (shown previously in Figure 1.5), vibrations propagating from the geophone to the tip undergo some level of attenuation and phase shift. The structure of the
2.1 Theoretical Background

STM between the geophone and tip dictates the unique transformation of vibrations at each frequency. To quantify this transformation, a calibration measurement of the geophone $G_c$ and tip $Z_c$ vibrations yields a transfer function $T(\omega)$. The calibration measurement is taken with the tip fixed in the XY plane with a constant bias and current. Equation 2.1 outlines the derivation of the transfer function, which involves the Fourier transformation ($\hat{\cdot}$) of both the tip and geophone signal and calculating the complex ratio (encoding the amplitude and phase shift) between the two at each frequency. Moreover, note that $Z_c$ and $G_c$ are discretely-sampled data and the Fourier transformation applied to the signals is a discrete-time Fourier transformation (DTFT). Various factors can affect the accuracy of the DTFT and the subsequent accuracy of the transfer function. An analysis of these factors can be found in Appendix A and the optimal parameters were used throughout the remainder of this thesis.

$$T_{Z}(\omega) = \frac{\hat{Z}_c(t)}{\hat{G}_c(t)}$$ (2.1)

This transfer function can then be applied to subsequent geophone signals during scanning and to estimate and reduce $Z$ noise at the tip. Equation 2.2 outlines such an application, with $G$ and $Z_n$ representing the measured geophone signal and estimated $Z$ noise. The ($^{-1}$) operator represents an inverse Fourier transformation. Figure 2.1 is an example of this process with the estimated $Z$ noise closely resembling the measured $Z$ noise. The estimated noise $Z_n$ can then be subtracted from the measured signal $Z_m$ to yield the original signal $Z_s$.

$$Z_n = \left(\hat{G}T_{Z}\right)^{-1}$$ (2.2)

$$Z_s = Z_m - Z_n$$ (2.3)
2.1 Theoretical Background

![Graph showing Z noise (blue), geophone signal (black), and estimated Z noise (green).](image)

**Figure 2.1:** Equations 2.1 and 2.2 can estimate Z noise using a transfer function and geophone signal. The measured Z noise (blue) exhibits noise at ∼56 Hz and the geophone signal (black) captures this information, although compounded with the resonance frequency of the geophone itself. After applying the transfer function to the geophone signal, the estimated Z noise (green) closely resembles the measured Z noise.

2.1.2 Spectroscopic Cancellation

Fundamentally, spectroscopic measurements are different from topographic data and require a different set of consideration for a successful cancellation scheme. Due to the weaker $dI/dV$ signal, a lock-in amplifier is used to extract the signal from the noisy environment. The lock-in amplifier modulates the bias $V(t)$, measures the current $I(V(t))$, and outputs the lock-in signal $LIY$ using Equation 2.4. The bias modulates according to Equation 2.5. This process yields several complications when attempting...
2.1 Theoretical Background

to reduce vibrational noise from the \( LIY \) signal.

\[
LIY = \frac{1}{T} \int_{t'}^{t'+T} I(V(t)) \cos(\omega t) dt \quad (2.4)
\]

\[
V(t) = V_{DC} + V_{AC} \cos(\omega t) \quad (2.5)
\]

First, vibrations exponentially affect the current signal (Equation 2.6) as spectroscopic data measurements are completed with the tip fixed at a spatial location and vibrations alter the tip-sample distance \( Z \). Second, the lock-in amplifier calculates the product of the current signal and the modulation function \( \cos(\omega t) \), which shifts the frequency of noise from \( \omega_n \) to \( \omega \pm \omega_n \). Finally, the integration of this product across the period of bias modulation \( T \) leads to a non-linear expansion of the noise frequency to \( \omega_n, \omega \pm \omega_n, 2\omega \pm \omega_n ..., \) with varying levels of attenuation. The overall complication of the lock-in amplifier with vibrational noise can be seen in equation 2.7. To account for these complications, this project took four different approaches to find the optimal spectroscopic noise cancellation method (see Table 2.1). An in-depth discussion of each approach can be found in Appendix B.

\[
I(Z_m) = I(Z_s) e^{-\kappa Z_n} \quad (2.6)
\]

\[
LIY = \frac{1}{T} \int_{t'}^{t'+T} I(V(t)) e^{-\kappa Z_n} \cos(\omega t) dt \quad (2.7)
\]

Of the four approaches, the G-LIY Direct approach is the optimal noise cancellation scheme. This approach makes two approximations. The first approximation (Equation 2.8) approximates the noise to a constant level throughout the period of a bias modulation, which extracts the noise term \( e^{-\kappa Z_n} \) from within the integral to a coefficient outside the integral. The assumption is only valid if the noise of interest
2.1 Theoretical Background

### Table 2.1: Four Approaches to Cancelling Spectroscopic Noise

<table>
<thead>
<tr>
<th>Description</th>
<th>Mechanics</th>
<th>Approximations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact Propagation</td>
<td>$G \rightarrow Z \rightarrow I \rightarrow LIY$</td>
<td>-</td>
</tr>
<tr>
<td>Z-LIY Propagation</td>
<td>$G \rightarrow Z \rightarrow LIY$</td>
<td>Equation 2.8</td>
</tr>
<tr>
<td>G-LIY Direct</td>
<td>$G \rightarrow LIY$</td>
<td>Equation 2.8 &amp; 2.9</td>
</tr>
<tr>
<td>G-log(LIY) Direct</td>
<td>$G \rightarrow \log(LIY)$</td>
<td>Equation 2.8</td>
</tr>
</tbody>
</table>

is at a significantly lower frequency than the frequency of the bias modulation. This is true for spectroscopic imaging, as most vibrational noise are below 120 Hz and the lock-in amplifier modulates bias at $\sim 1.1$ kHz. The second approximation (Equation 2.9) approximates the exponential effects of distance on current to a linear relationship. This is based on the Taylor expansion $e^x = 1 + x + \frac{x^2}{2!} + ...$ given that $x$ is sufficiently small (i.e. the vibrations have a small amplitude on the order of picometers with $\kappa \approx 10^{15}$). The resulting combination of both approximations in Equation 2.10 suggests a transfer function can be calibrated directly between the geophone signal and $LIY$ signal with the tip feedback disengaged.

$$LIY = \frac{1}{T} \int_{t'}^{t'+T} I(V(t)) e^{-\kappa Z_n} \cos(\omega t) dt \approx e^{-\kappa Z_n} \frac{1}{T} \int_{t'}^{t'+T} I(V(t)) \cos(\omega t) dt \quad (2.8)$$

$$I(Z) = I(Z_0) e^{-\kappa Z_n} \approx I(Z_0) (1 - \kappa Z_n) \quad (2.9)$$

$$LIY_m \approx LIY_s (1 - \kappa Z_n) \quad (2.10)$$

Although equation 2.10 may have a similar form to equation 2.3, the calibration and application of a transfer function between $G$ and $LIY$ must account for the $LIY_s$ coefficient on the right hand side. $LIY_s$ is dependent upon a host of factors, including the sample material, bias, and current. Therefore, it is not feasible to
calculate a transfer function for each $LIY_s$ value, but rather calibrate a single transfer function between the geophone signal $G$ and a $LIY_c$ signal divided by its mean $\overline{LIY_c}$ in equation 2.11. The transfer function is then applied to a geophone signal $(\tilde{G}T_{LIY})^{-1}$ during a bias spectroscopy before scaling by $LIY_m$ as an estimation of $LIY_s$ at each corresponding bias value. The result of this calculation can then be subtracted from the measured $LIY$ signal ($LIY_m$) for the noise-reduced $LIY_s$ signal as shown in 2.12. Note the change from + to − in the equation as the transfer function $T_{LIY}$ encodes this information during the calibration process.

$$T_{LIY}(\omega) = \frac{LIY_c/\overline{LIY_c}(t)}{\tilde{G}_c(t)}$$  \hspace{1cm} (2.11)

$$LIY_s \approx LIY_m + LIY_s\kappa Z_n = LIY_m - LIY_m (\tilde{G}T_{LIY})^{-1}$$  \hspace{1cm} (2.12)

## 2.2 System Implementation

This section will cover the implementation of the theoretical noise cancellation scheme alongside Nanonis, the native STM controller software. Section 2.2.1 gives an overview of the user interaction with the system and connections between different components within the system. Section 2.2.2 and 2.2.3 follows with an in-depth explanation of the mechanics of each custom-built component.

### 2.2.1 Overall System

Presently, researchers initiate a topographic scan on the STM through the Nanonis Scan Monitor which automatically produces topographic scan images. To ensure minimal disruption to the present workflow of STM users, the implemented noise cancellation scheme must minimize the number of steps required to produce the same
2.2 System Implementation

![System architecture diagram]

**Figure 2.2: System architecture to simplify user interaction between the Nanonis software, LabVIEW, and Python.** The green pathway shows how to calibrate the transfer function: the user executes the calibration from LabVIEW, which calls the Nanonis Data Logger module to record calibration data before the Python script generates and saves a calibrated transfer function. The blue pathway represents the noise-cancellation of topographic images, with the user executing a scan through the LabVIEW UI. This calls the Data Logger and Scan Monitor modules and runs the cancellation Python script once the scan is completed. The resulting raw topographic image can be used verify the accuracy of the cancellation script by comparing the raw image from the script to the image from the Scan Monitor module. The processed (and raw) image is saved as a 2D numerical array for easy access and further analysis.

topographic scan image. This is achieved through a simple LabVIEW front-end (in Figure 2.3 below) coupled with a calibration and a cancellation Python script, which automatically generates a raw and processed topographic image. The LabVIEW interface allows the user to either “calibrate” or “scan” and executes the calibration and cancellation pathway respectively. When the “Calibrate” toggle is selected, the LabVIEW program calls the Nanonis Data Logger to record $G$ and $Z$ with the tip in feedback. Subsequently, when the user deselects the “Calibrate” toggle, the Lab-
VIEW program halts the data collection and executes the calibration Python script to calculate the transfer function from the collected data. After calibration, the user can set the appropriate scanning parameters in Nanonis Scan Monitor as he or she would in the present workflow except for the scan initiation, which would occur with the selection of the “Scan” toggle. The “Scan” toggle also initiates the data logger module to collect X, Y, Z coordinate and geophone data as the scan progresses. The LabVIEW program then halts data collection, executes the cancellation Python script, and deselects the “Scan” toggle once the scan is completed. The output files from the Python script includes a pre-processed image and a noise-cancelled image.

2.2.2 LabVIEW Program

Figure 2.3: A minimal user interface in LabVIEW. A simple user interface automates the complex post-processing method for users through the back-end and external Python scripts. The LabVIEW user interface consists of the calibrate switch which turns the data logger on and off for calibration and a scan switch to initiate scanning. The direction toggle dictates the direction of the scan and the stop is an emergency stop which would halt the LabVIEW program.
2.2 System Implementation

The LabVIEW program serves as the user interface and command center for the Nanonis modules and Python scripts. LabVIEW was chosen as the programming language for this module due to two reasons: the graphical user interface and a Nanonis-built programming interface. LabVIEW is a visual programming language with a Front Panel and a Block Diagram coding canvas. This allows for a rapid construction of a clean UI front end with the appropriate connections to the logical processes in the back end. Furthermore, Nanonis developed a LabVIEW programming interface such that any program can measure, modify, and execute functions available within the existing STM controller software. The programming interface allows the LabVIEW program to sequentially execute functions within the STM controller and measure key scan parameters pertinent to the Python scripts. Auxiliary functions within LabVIEW, such as the connection to command prompt, ensure automated, successful file transfers between Nanonis modules and the Python scripts while minimizing storage space usage.

2.2.3 Python Scripts

The calibration Python script consists of loading the data files, processing the data, and saving a transfer function. To load the appropriate data files, the Python script uses a file naming and format convention in agreement with the Nanonis Data Logger output files. The loaded data is then passed through several functions, which account for tip changes and thermal drifting as seen in Figure 2.4, before calibrating a transfer function based on Equation 2.1. The transfer function is stored as an array of frequencies and complex numbers under a file naming convention consistent with the LabVIEW program and the cancellation Python script.

The cancellation Python script follows the same structure as the calibration Python script. The script loads the scan data and transfer function from the Nanonis Data
2.2 System Implementation

Figure 2.4: Detecting and eliminating tip changes and thermal drifting. Tip changes can be seen as sharp increases or decreases in the raw $Z$ signal on the left graph. Thermal drifting contributes to a gradual sloping background in the right graph, well captured by a second-degree polynomial. Both effects are taken into account of before calibrating a transfer function.

Logger module and from the calibration Python script. Data processing involves finding $Z_n$ from the geophone data and transfer function, binning each $Z_m$ and $Z_s$ data sample using the X and Y coordinate to the corresponding pixel in the raw and processed images, and outputting the final images based on the average pixel values. The images are then stored as a 2D array of values for researchers to easily access and analyze the results.
Chapter 3

Topographic Noise Cancellation

Summary

The topographic noise cancellation scheme was tested under both standard operating conditions and noisy conditions to evaluate the effective topographic noise reduction. Section 3.1.1 describes the measurements and analysis of ambient noise reduction and concludes the scheme achieved 20.9% ± 3.6% RMS noise reduction. Similarly, Section 3.1.2 gives the measurements and analysis under a driven noise condition and concludes the scheme achieved 81.5% ± 6.4% RMS noise reduction. Pre-processed and processed topographic images are examined in Section 3.2 under both ambient and driven noise conditions to visually demonstrate the impact of the post-processing scheme.
3.1 Effective Noise Reduction

3.1.1 Ambient Noise Reduction

To quantify the ambient noise reduction, a calibration measurement (described in Section 2.1.1) was taken over the course of 40 minutes under standard operating conditions. The standard operating conditions for the STM include activated pneumatic isolators, a sealed anechoic chamber, a vacuum environment within the STM, and a filled liquid Helium dewar. The software settings for the STM include PI controller parameters of $P = 5 \text{ pm}$ and $I = 60 \text{ m/s}$, current set point of 500 pA, and a bias of 500 mV. This continuous data is then segmented into a training and test data set, where the training set is used to calibrate the transfer function and the test set is used to measure the ambient RMS noise and RMS noise reduction with the transfer function. The training set consists of five 20-minute long segments (using overlapping elements i.e. 0-20 min, 5-25 min, 10-30 min etc.) to calibrate 5 different transfer functions. The test set consists of ten 50-second long segments spaced evenly apart throughout the calibration measurement. The noise cancellation scheme is applied to each test segment using each of the 5 different transfer functions. From the RMS noise value pre- and post-processing, the mean reduction in RMS noise is $20.9\% \pm 3.6\%$ from 155 fm to 123 fm. A keen observer may note that the % reduction is less than the % reduction recorded by Primavera (48% from 683 fm to 353 fm), but his observations were in a noisier environment and the post-processed RMS value is greater than this report’s observed values. Furthermore, a paired T-test between the pre-processed and post-processed RMS values yields a $p$ value of $2.2 \times 10^{-50}$, which suggests the theoretical work described in Section 2.1.1 significantly outperforms a random signal-processing scheme in reducing RMS ambient noise. This can also be seen in Figure 3.1, where the measured signal (blue) in the background can be seen...
3.1 Effective Noise Reduction

Figure 3.1: A 20.9% reduction in ambient noise between the measured and processed Z trace. This is an example of a 50-second long test segment using one of the five transfer functions. The other transfer functions performed similarly across all test segments.

with larger variations than the processed signal (orange) in the foreground. In an ideal noiseless environment, the Z signal should be a line at 0 pm across the time domain.

As outlined in Section 1.5, the target noise attenuation bandwidth is 0-300 Hz and the analysis in the previous paragraph does not capture this information. To examine the noise attenuation across the frequency domain, the DTFT of the test segments pre- and post-processing converts the noise from the time to frequency domain in Figure 3.2. The peaks above the base noise level (which is mainly $1/f$ pink noise) represent noise detected at the tip. The blue processed signal clearly attenuates most peaks across the 0-300 Hz when compared to the red measured signal. In addition, most vibrational noise occur between 40 and 80 Hz (emphasized in the inset plot)
Figure 3.2: Successful attenuation of ambient topographic noise across the designed bandwidth. The desired bandwidth is 0-300 Hz, represented by the blue dashed line. The frequency plot shows a baseline pink noise with sharp peaks representing vibrational and electrical noise. Most noise are within the 40-80 Hz range. A closer look in the inset plot demonstrates an effective attenuation of most vibrational noise, with no attenuation of electrical noise at 60 Hz as that is out of the scope of this project.

with a clear peak at 57 and 60 Hz. The noise cancellation scheme significantly reduces the 57 Hz noise peak, which is attributable to vibrational noise, whereas the 60 Hz peak is relatively untouched as it is attributable to electrical noise. Therefore, the scheme is successful in attenuating ambient topographic noise across the specified bandwidth.

3.1.2 Driven Noise Reduction

The design specifications also outlines the need to evaluate the performance of the noise cancellation scheme under a driven-noise environment. As such, a 20” box fan was placed atop the STM table and switched on, while all other conditions were maintained equivalent to those in the prior section. Figure 3.3 depicts this setup.
3.1 Effective Noise Reduction

Figure 3.3: Driving noise in the STM with a box fan. The 20” box fan is placed on the wooden table and switched on to the lowest setting. Imbalances and imperfections of the box fan generates vibrational noise near the circuit frequency of 60 Hz.

within the STM room, which was expected to generate noise around 60 Hz and other frequencies due to imbalances within the fan and natural resonances of the STM. Measuring the driven noise reduction involved the same procedure from the prior section. A calibration measurement was taken over a course of 40 minutes. A training and test set was taken from the data and used to quantify the level of noise attenuation achieved.
3.1 Effective Noise Reduction

Figure 3.4: A 81.5% reduction in driven noise between the measured and processed Z trace. Note the driven vibrations recorded in the blue trace are somewhat coherent (the frequency slightly changes over time). The processed signal suppresses most of the driven vibrations and accounts for variations in amplitude and phase of the vibrations.

Figure 3.5: Successful attenuation of driven topographic noise across the designed bandwidth. Similar to Figure 3.2, the frequency plot shows a baseline pink noise but with larger vibrational peaks up until 300 Hz (blue dashed line). Note the significant reduction of the lower (20-40 Hz) and higher frequency peaks (above 200 Hz). There are several noise peaks which were not attenuated, which are mainly electrical noise and the higher harmonics.
The scheme reduced the RMS driven topographic noise by 81.5% ± 6.4% from 4402 fm to 785 fm. A paired T-test between the measured RMS noise and the processed RMS noise confirmed the noise reduction scheme significantly reduced the driven noise with a $p$ value of $6.5 \times 10^{-29}$. Inspection of the time traces of the measured and processed Z signals, as seen in Figure 3.4, also suggests a high level of noise attenuation. Furthermore, the fewer and lower peaks in the processed signal in Figure 3.5 compared to the peaks in the measured signal indicates the noise attenuation spans 0-300 Hz, as per the design specifications. Hence, the same noise attenuation scheme can reduce both ambient and driven vibrational noise.

3.2 Topographic Scan Results

After determining the noise cancellation scheme works well under both ambient and driven conditions, the application of the scheme is only useful for STM users when applied to topographic scan images. This requires the raw topographic image from the Python script to match the present image output from Nanonis. Several scanning sessions on the STM produced multiple topographic images, which were then used to compare against the scan file produced from Nanonis Scan Monitor (see Figure 3.6). Although the Python and Nanonis images are visually similar, a thorough investigation of the differences between the images was conducted. The quantitative analysis consists of subtracting each pixel value in the Nanonis image from the corresponding pixel value in the Python image and examining the spatial distribution of errors (see right image of Figure 3.7). A histogram, left in Figure 3.7, grouped similar pixel error values together to understand the value distribution of errors. Moreover, to be consistent with the RMS noise calculations in prior sections, the overall RMS pixel error between the two images was calculated and found to be 28 fm, which is less than the RMS noise attenuation attained by the noise cancellation scheme. However, the
3.2 Topographic Scan Results

Figure 3.6: No visible differences between Python- and Nanonis-generated topographic scans. The left image is generated from the cancellation Python script and the right image is the Nanonis image. The little difference between both images validates the logical process within the cancellation Python script.

Figure 3.7: Pixel error values between images in Figure 3.6 are within 0.2 pm. The image (right) represents the pixel error at each pixel location (in pm) between the Nanonis- and Python-generated topographic images. The histogram (left) counts the number of pixels (in log scale) with the corresponding pixel error values. Most values are within a 3 fm error as seen in the sharp peak in the center and the standard deviation of the distribution is $\sigma = 28$ fm.
3.2 Topographic Scan Results

structured distribution of the large errors within the error image suggests the pixel value error is a systematic rather than random error. Although no further reduction in this error was attained in this project, Section 5.2 outlines potential sources of this systematic error and how to address the issue in future work.

Given the raw image in the cancellation Python script matches the Nanonis output image, the noise cancellation scheme can then be applied to the topographic scan to compare between the pre- and post-processed images. The cancellation Python script was tested in both ambient and driven conditions and the resulting topographic images can be found in Figures 3.8 and 3.9. The processing time of the Python script varied between 1 to 5 minutes for scan images with up to $10^7$ data points (roughly a 13 minute scan at 10 kHz sampling rate). Under standard operating conditions, the post-processed image on the right does not significantly differ from the pre-processed image on the left. This is likely due to the low level of ambient noise in the STM relative to the signal from atomic features of the sample (roughly 0.1 pm noise versus 1 pm signal). However, there are significant differences between the pre- and post-processed images under the driven noise conditions. The topographic image was taken under the same setup as described in Section 3.1.2. The driven noise is significantly greater than the signal from atomic features of CeSb, leading to a saturated, pre-processed image with no atomic resolution in Figure 3.9. The post-processed image, on the other hand, achieves atomic resolution with the noise cancellation scheme attenuating driven noise and revealing the underlying atomic lattice of the sample. Attaining atomic resolution imaging in the noisy setup suggests the operating conditions for the STM could expand to tolerate higher vibrational noise at the tip.
3.2 Topographic Scan Results

Figure 3.8: Little difference between the pre- and post-processed topographic images under ambient conditions. The pre-processed image (top) already achieves atomic resolution, with darker regions on the brighter lattice representing atomic defects within the atomic lattice of CeSb. The post-processed image (bottom) is visually similar to the pre-processed image and does not provide any additional information. Note that both images have occasional horizontal lines, which represent changes in the bi-stable tip during scanning rather than actual topographic features.
3.2 Topographic Scan Results

Figure 3.9: Noise reduction scheme enables atomic-resolution topographic imaging in noisy environments. The pre-processed image (top) has saturated striations that represent the driven noise caused by a fan on the table, which changes phase and frequency throughout the scan. The post-processed image (bottom) significantly attenuates the driven noise and gives an atomic-resolution image with the lattice structure and regions of defects clearly shown. Both images are on the same color scale of -2 to 2 pm.
Chapter 4

Spectroscopic Noise Cancellation

Summary

The spectroscopic noise cancellation scheme was tested under both standard operating conditions and noisy conditions to evaluate the effective spectroscopic noise reduction. Section 4.1.1 describes the measurements and analysis of ambient noise reduction, but the results were inconclusive due to significant electrical noise in the system. However, Section 3.1.2 gives the measurements and analysis under a driven noise condition, which amplifies the vibrational noise relative to electrical noise and concludes the scheme achieved a $65.4\% \pm 8.7\%$ RMS noise reduction.

4.1 Effective Noise Reduction

4.1.1 Ambient Noise Reduction

In the same way Section 3.1.1 quantified ambient noise reduction, the process for calculating the ambient noise reduction in spectroscopic data involves a calibration measurement between the geophone and LIY signal under standard operating con-
4.1 Effective Noise Reduction

ditions. Since the tip is not in feedback, thermal drifting prohibits the calibration measurement from proceeding continuously for a long period of time as this would risk crashing the tip into the sample. Hence, only 2-minute long measurements were recorded on the STM, segmented into training and test data sets, and used to calibrate and assess the spectroscopic noise reduction. Following the scheme outlined in Section 2.1.2, a transfer function was calibrated between the geophone and LIY signal over the training data (100 seconds) and applied to the test data (20 seconds).

The tests did not demonstrate significant reduction in ambient noise. Time traces between the measured and processed spectroscopic signals in Figure 4.1 show no reduction in the overall noise. However, a plot of the signal in the frequency domain in Figure 4.2 reveals the reason for the seemingly ineffective noise cancellation. The white noise apparent in the frequency domain is attributed to electrical noise from three areas of the STM circuit: shot noise, Johnson noise, and voltage noise. With a bias across the tip-sample junction, electrons tunnel through the junction and this movement is the tunneling current and the measured LIY. This leads to shot noise as the discrete electrons tunnel across the junction according to a Poisson distribution. As current flows through the circuit, the current fluctuates due to thermal excitation of the electrons. This is Johnson noise and can be quantified based on the 1GΩ resistor in the current amplifier. The circuit also includes amplifiers for the measured current, which is susceptible to voltage noise at the amplifier source. These three electrical noise sources explains the baseline white noise of $\sim 20 \, \text{fA Hz}^{-1/2}$ seen in the frequency plot. Despite the white noise, a sharp vibration peak at 57 Hz and other noise peaks around 60 Hz can be seen in the inset plot. A spectrogram in Figure 4.3 examined the evolution of these peaks across the time domain and implied the coherent noise peak at 57 Hz is likely a mechanical vibration and the incoherent noise peaks around 60 Hz is likely electrical noise. The noise cancellation scheme successfully reduces the 57 Hz peak in the processed data and did not reduce the 60 Hz noise.
4.1 Effective Noise Reduction

Figure 4.1: No visible reduction of ambient spectroscopic noise in time trace. The processed LIY in the foreground matches the measure LIY in the background in noise amplitudes. Most noise within the spectroscopic signal is electrical rather than vibrational noise.

Figure 4.2: The processed signal reduces a 57 Hz vibration peak despite high levels of electrical noise. The white noise baseline is a combination of Shot, Johnson, and voltage noise. Although the electrical noise masks many vibrational noise, a peak at 57 Hz is likely attributed to vibrations from nearby cryopumps and was successfully reduced in the processed signal.
Figure 4.3: The vibration peak at 57 Hz remains coherent whereas the electrical noise at 60 Hz is incoherent and aliasing. As the ambient LIY was measured, the electrical noise at 60 Hz devolves to two frequencies and explains why the electrical noise at 60 Hz in Figure 4.2 is a broad peak rather than a sharp peak. The cancellation of 57 Hz and not the 60 Hz peaks bolsters the validity of the noise cancellation scheme since the scheme only detects and cancels vibrational, rather than electrical, noise.
4.1 Effective Noise Reduction

4.1.2 Driven Noise Reduction

To further verify whether the noise cancellation scheme works for spectroscopic imaging, vibrational noise must be detectable and greater than electrical noise. Using the setup of a box fan on the wooden table (same as in Figure 3.3), vibrational noise in the STM would increase beyond the electrical noise. A 200-second long measurement of LIY was recorded with the box fan running on the STM table. As the 200-second long data segment is significantly shorter than the 40-minute long data segment collected for topographic scanning, a different treatment of the data is necessary to produce meaningful results. The 200-second long data was segmented into a 180-second training data set and a 20-second test data set. The training data set yielded a transfer function between the geophone and LIY signal and the test data set evaluated the RMS noise reduction of the transfer function. This process was repeated ten times using different combinations of training and test data sets (i.e. test data set from 0-20 seconds, 20-40 seconds...180-200 seconds of the original trace). Across the ten different tests, the noise cancellation scheme achieved a 65.4% ± 8.7% reduction in RMS noise from 2982 fA to 970 fA. A paired T-test between the pre- and post-processed RMS values of the ten test segments reported a $p$ value of $4.0 \times 10^{-5}$. This confirms the scheme significantly reduces LIY vibrational noise across the specified 0-300 Hz bandwidth. This is evident in both Figures 4.4 and 4.5, where the measured LIY has significantly higher fluctuations than fluctuations in the processed signal in the time trace and most noise peaks in the measured signal are reduced in the processed signal in the frequency plot.
4.1 Effective Noise Reduction

Figure 4.4: The noise cancellation scheme successfully attenuates the driven vibrational noise in the measured LIY signal. The fluctuations in the measured LIY signal under noisy conditions are greater than that under ambient conditions. The scheme significantly reduces the LIY RMS noise by 65.4% ± 8.7% and the processed LIY fluctuations have a similar magnitude to the fluctuations found under ambient conditions.

Figure 4.5: Attenuating most vibrational noise peaks to the baseline electric noise in spectroscopic data. The noisy environment generated more vibrational peaks above the white noise in the measured signal compared to that in Figure 4.2. The processed signal reduced most of these peaks up to 300 Hz (dashed blue line) and particularly in the 40-80 Hz range. Note grounding noise at 60 Hz and higher harmonics is apparent in both the measured and processed noise.
Chapter 5

Conclusions

The STM is an atomic-resolution microscope that can collect sensitive topographic and spectroscopic data from a sample. These measurements are highly susceptible to vibrations as features of interest are on the scale of picometers and picoamperes. The post-processing method outlined in this thesis quantifies how vibrations affect measurements and then subsequently reduces noise in measurements by recording the vibrations within the STM. Analyses of the performance of the system concluded significant vibrational noise reductions were achieved in topographic and spectroscopic data under ambient and noisy conditions. The post-processing method can further reduce vibrational noise, improve the signal strength, and reduce the scanning time or enlarge the scanning area. Future work to improve the solution include reducing the error between the Nanonis and Python generated topographic images, testing the spectroscopic noise cancellation under ambient conditions and lowered electrical noise, and improving the transfer function to account for non-linear vibration propagation. As the post-processing method can be combined with passive vibration isolation systems and requires minimal hardware changes to the existing equipment, there are also possible applications of this post-processing method to other sensitive measurement equipment as a low-cost vibration mitigation system.
5.1 Project Success

Overall, the solution successfully met the initial specifications in reducing vibrational noise across topographic and spectroscopic data under ambient and noisy conditions. The scheme reduced topographic vibrational noise by 20.9% ± 3.6% in ambient conditions and by 81.5% ± 6.4% in driven noise conditions. Although the scheme did not achieve the target noise reduction of > 80% under ambient conditions, the scheme did achieve > 80% noise reduction in driven noise conditions. For spectroscopic vibrational noise, the scheme reduced a 57 Hz vibration peak under ambient conditions, but white, electrical noise masked most vibrational noise and the results were inconclusive. In addition, the scheme achieved a 65.4% ± 8.7% reduction of driven spectroscopic noise. The noise attenuation in topographic and spectroscopic data spanned the specified 0-300 Hz bandwidth. The system’s implementation with a LabVIEW user interface and Python back-end also ensures the vibration mitigation scheme can be easily used by researchers to improve the effective noise isolation of the STM. Finally, the Python back-end executes immediately following a scan and completes the scanning procedure within 5 minutes, which is close to the initial specifications for a simultaneous execution of the algorithm. The solution fulfills some of the initial specifications, but also makes significant headway towards the target noise reduction levels.

5.2 Future Work

To further improve the solution and achieve all the initial design specifications, future work could tackle three main areas of the project: accounting for non-linear responses in the transfer function, reducing the error between the Nanonis and Python topographic scans, and using an alternative approach to cancel spectroscopic vibrational noise.
First, a nonlinear transfer function could potentially improve noise attenuation in topographic and spectroscopic data. Presently, a transfer function from the geophone to the tip assumes a linear propagation of vibrations through the structure between the two locations. However, the STM arm is a mechanically complex system and could exhibit nonlinear behaviors. As such, vibrations detected at one frequency from the geophone could cause vibrational excitation at other frequencies at the tip. In addition, spectroscopic data exhibits nonlinear frequency propagation as the lock-in amplifier shifts low frequency vibrations towards the lock-in frequency (see Figure 5.1). Hence, a multi-layered, sigmoid neural network could account for linear and nonlinear frequency propagation.

![Figure 5.1: Low frequency vibrations shifted towards the lock-in frequency.](image)

The lock-in amplifier shifts low frequency vibrations at $\sim 60 \text{ Hz}$ (left plot) towards $\sim 1260 \text{ Hz}$ (right plot) with a bias modulation frequency of 1200 Hz. Note a mirror of the $\sim 1260 \text{ Hz}$ is also apparent in $\sim 1140 \text{ Hz}$. A nonlinear transfer function can account for the effects of the lock-in amplifier.

Second, Figure 3.7 outlined pixel value errors between the Nanonis- and Python-generated topographic images. The error image (right of the same figure) demonstrates that large pixel error values are concentrated within the upper-left and lower-right corners of the image, which implies a systematic error exists between Nanonis and the Python code. A likely reason for the systematic error is the different spatial coordinate information given to Nanonis and Python. In order to scan a topographic
image, the software must direct the tip to scan across the image using piezoelectric devices. A digital-analog converter translates the digital $X$ and $Y$ coordinates to an analog $X'$ and $Y'$ signal for the piezoelectric devices. The DAC has a 20-bit resolution, which gives a 0.38 pm resolution across the 400 nm scan area. If $dX$ is not commensurate with multiples of 0.38 pm, the analog output will not have a constant $dX'$, but rather periodically increase or decrease one $dX'$ value by 0.38 pm such that the overall $\Delta X'$ is consistent with $\Delta X$. This can be problematic since the Nanonis-generated image places measurements in their respective pixels based on $X$ and $Y$, whereas the Python script can only access $X'$ and $Y'$ to place measurements in the appropriate pixel. Further investigation and correspondence with Nanonis engineers could shed light onto this issue. There may be a set of scan settings in which the systematic error would not be present and this scheme may be restricted to scan within those settings. Alternatively, building a system with direct access to the analog-digital converter could reduce (or remove) discrepancies between the Nanonis- and Python-generated topographic images.

Third, there may be potential to reduce spectroscopic noise further using one of the alternative approaches outlined in Table 2.1. The present implementation of spectroscopic noise cancellation relies upon two approximations. An exact propagation approach does not require these approximations and could lead to a higher level of noise attenuation. However, this approach requires an accurate implementation of the lock-in amplifier. Nanonis implements the lock-in amplifier within the controller’s FPGA, which has direct access to the 1 MHz analog-digital converter data stream and the reference sine wave. Presently, the Python script only has access to the 20 kHz down-sampled data stream and a measurement of the reference sine wave. These two factors could lead to discrepancies between the Python and Nanonis lock-in amplifiers and hamper the overall noise reduction levels. Future work could explore accessing the 1 MHz data stream within the Nanonis controller to accurately imple-
ment the lock-in amplifier and enable the exact propagation approach to cancelling spectroscopic noise.
Appendix A

Optimal Transfer Function

Introduction

Figure A.1: Four different calibration parameters that affect the transfer function. The performance of a transfer function depends on the calibration duration, segment length, segment overlap, and Kaiser window parameters. The blue bars represent data samples, with time represented as the horizontal axis and overlap between segments containing the same data samples.

There are four parameters which can affect the efficiency of a transfer function, as outlined in Figure A.1. First, the total duration of the calibration measurement can affect the transfer function and overall performance of the solution. If the calibration duration...
duration is too short, noise within the measurements will skew the transfer function and subsequent applications in the cancellation scheme. If the calibration time is too long, incremental calibration measurements beyond the threshold for a clean transfer function would not be necessary and waste valuable time on the STM for data collection. Second, the segment size of data used in equation 2.1 (reproduced below) must also be optimized. Since a calibration measurement can take upwards of 30 minutes, the data can contain more than 18 million data samples and calculating the transfer function would be computationally taxing if used in its entirety. Instead, the data can be separated into smaller segments, with each segment producing a transfer function and the overall transfer function an average of those transfer functions. The length of the segments dictates the frequency resolution of the transfer function based on $1/T$, where $T$ is the time length of a segment. Longer data segments can yield better frequency resolutions but also require a longer computation time.

\[
T_Z(\omega) = \frac{\tilde{Z}(t)}{G(t)} \quad \text{(A.1)}
\]

Averaging over numerous transfer functions also reduces noise within the overall transfer function. Longer segments would have less segments to average relative to shorter segments over the same duration. To further improve averaging of transfer functions, more segments can be generated from a measurement by overlapping neighboring segments with identical data samples. The increased number of segments allows for more averaging, although there will exist a number of segments where additional segments generated will not yield further improvements as they fundamentally contain the same data samples (i.e. the extreme case where each subsequent segment shifts along the measurements by one data sample). The final parameter is the Kaiser window parameter that governs the window function applied to each segment prior to the DTFT. A window function serves to mitigate aliasing and spectral leakage and
different windowing parameters affect the spectral leakage in different ways.

To find the optimal parameters, the different parameters were tested independently using a similar testing method to the testing outlined in Section 3.1.1. The data consists of 40-minute long measurements of the geophone and Z signal. Then, ten 50-second long segments evenly spaced apart across the measurements were earmarked for testing and excluded from the training set. The training set is used to calibrate different transfer functions based on the range of parameter values. The % RMS noise reduction of each transfer function is then evaluated on every testing segment to determine the optimal parameter value. The comparison is also completed visually using a box-and-whisker plot. After visual inspection of the plot, a paired-T test is also conducted between the result sets of neighboring parameter values to ensure there would be no significant improvements in % RMS noise reduction when moving away from the optimal parameter value (where significance is defined as \( p < 0.05 \)).

A.1 Calibration Duration

Intuitively, longer calibration duration should yield better noise reduction results as more time allows for more averaging and a stronger signal. However, testing calibration duration between 250 and 2500 seconds under ambient and noisy conditions demonstrate this is not necessarily true. The results (Figures A.2 and A.3) show a plateau in noise reduction for transfer functions with a calibration duration greater than 1000 seconds. In the ambient conditions test, the optimal calibration duration was 1500 seconds, based on the mean % RMS noise reduction across the test segments. This was reduced to 1250 seconds under noisy conditions as the driven noise likely produced a stronger ‘signal’ regarding the attenuation and phase shift of vibrations. Also note the mean % RMS reduction only differed by < 1% across
A.1 Calibration Duration

Figure A.2: Optimal calibration duration is 1500 seconds in ambient conditions. The plateau beyond 1000 seconds of calibration suggests minimal gains in the % RMS reduction, with the 1500-second transfer function producing the greatest mean % RMS reduction. In this plot and subsequent box-and-whisker plots in this appendix, the mean and median % RMS reduction value is shown with a green triangle and an orange horizontal line respectively. The ends of the boxes represent the first and third quartile range and the whiskers represent the maximum and minimum non-outlier data point. Outliers are identified with ‘x’ and are calculated as values that are 150% the interquartile range below the first or beyond the third quarter.

calibration durations from 1000 to 2500 seconds and the paired-T tests confirm the differences are insignificant as the $p$ values between those test result sets were greater than 0.25. Therefore, calibration measurements should be at least 1250 seconds long and any additional calibration time beyond that point does not yield better results. Furthermore, since similar conclusions could be drawn from both ambient and noisy conditions, the remainder of the analysis will only inspect results under ambient conditions.
Figure A.3: Optimal calibration duration is 1250 seconds in noisy conditions. The same plateau identified in Figure A.2 above can also be found in % RMS reduction under noisy conditions. The slightly shorter calibration time is likely due to the significant attenuation/phase shift ‘signal’ generated by the fan.

A.2 Segment Length

The segment length dictates the frequency resolution of the transfer function as well as the amount of averaging possible from a given set of data. To find the optimal segment length, the % RMS noise reduction test was conducted between segment lengths of 5 to 50 seconds. Figure A.4 demonstrates some variations in the % RMS reduction across the segment lengths, although no clear trend can be identified. A paired-T test also showed no significant differences across the entire range of segment lengths. The highest mean % RMS reduction was achieved with a transfer function using 15-second-long segments. However, the maximum frequency resolution of the transfer function is inversely proportional to the segment length and a higher frequency resolution is desirable. Therefore, the 25-second-long segment length would yield an optimal transfer function for the increased frequency resolution and a similar % RMS reduction.
Figure A.4: 25-second-long segment length yields an optimal transfer function. Although the mean % RMS reduction is slightly lower (21.7%) than that of the 15-second-long group (21.8%), the increased frequency resolution from a longer segment length justifies the trade-off for an optimal transfer function.

Figure A.5: No significant differences in % RMS reduction between different Kaiser window parameter values. A window parameter value of 4 yields a slightly higher mean % RMS reduction, but any value would yield an acceptable transfer function.
A.3 Kaiser Window

The Kaiser window parameter defines the windowing function for each segment. A windowing function addresses spectral leakage and aliasing by skewing the weighting of each sample before DTFT. The Kaiser window heavily weighs the center while lessening the weighting on the start and end of a data segment. The parameter alters the shape of the function and consequently the ratio of weighting between the middle and ends of the segment. Typical values for the parameter are in the single digits and the testing covers a similar range from 0 (no windowing) to 9. Similar to segment lengths, the results and paired-T tests show no significant differences across the range of parameter values in Figure A.5. A slightly better % RMS reduction was achieved by a window parameter value 4. Therefore, any window parameter would be acceptable with a slight preference towards a Kaiser window parameter of 4.

A.4 Segment Overlap

The duration of a segment overlap is the number of identical samples shared between neighboring segments. Segment overlap allows for more segments and more averaging to be derived from a fixed length of measurement for a stronger signal in the transfer function. However, too many segments would undermine the original purpose of segmentation: faster computation. An overlap of between 1 and 10 seconds was used in testing and the results confirm that more overlap leads to a better transfer function (see Figure A.6). Paired-T tests between result sets yielded p values greater than 0.5, which suggests the differences between overlap values are insignificant. For an optimal transfer function, it may be best to use the maximum reasonable overlap of 10 seconds.
A.4 Segment Overlap

Figure A.6: Greater segment overlap gives a better transfer function with Kaiser windowing. There is a slight increase in mean % RMS reduction as the segment overlap duration increases. A segment overlap of 10 seconds within a 25-second-long segment length means all but a few data samples will be in two data segments for averaging.

Conclusion

Various parameters were tested independently based on the level of noise attenuation attained through the resulting transfer functions. In this analysis, the calibration duration, segment length, and segment overlap had the most impact on the overall performance of transfer functions. The recommended settings for an optimal transfer function is a 1250 seconds-long calibration process with 25-second-long segments and 10-second-long overlap between segments with an optional Kaiser window parameter of 4. This being said, as the testing of each parameter was conducted independently, one may find another optimal transfer within the four-dimensional parameter space which was not covered in this analysis.
Appendix B

Spectroscopic Noise Approaches

Introduction

As outlined in Section 2.1.2, there are four approaches to cancel vibration noise in the spectroscopic data. Theoretically, the exact propagation approach should lead to the best results as no approximations or assumptions are made. However, in practice, an exact propagation approach faces multiple implementation challenges. Therefore, the three other approaches make some approximations to circumvent these implementation challenges, with the G-LIY direct approach yielding the best results. In this chapter, the results of each approach will be shown alongside a discussion of the drawbacks of the approach.

B.1 Exact Propagation

For this approach, the exact propagation is based upon the theoretical background of the lock-in amplifier in Equation B.1. This requires three intermediate steps before the geophone signal can be converted to LIY noise. First, the geophone signal is transformed to Z noise using a topographic transfer function. Then, the Z noise is extrapolated to current noise using the $I \propto e^{-\kappa Z}$ relation. In the final step, the current noise is incorporated into a digital lock-in amplifier and produces the noise-
Figure B.1: Z spectroscopy experimentally determines $\kappa$. By withdrawing the tip from the sample in the Z direction, the measured current gives a logarithmic relationship to Z, which is used to determine $\kappa$.

cancelled LIY signal. In practice, the first two steps are easy to implement - the first step is identical to topographic scans and the second is an exponential with a time-independent $\kappa$, which can be experimentally determined as shown in Figure B.1. The results of the first two steps is shown in Figure B.2, where vibrational noise from the fan is seen in the current channel and the processed signal reduces a significant portion of vibration noise.

$$LIY = \frac{1}{T} \int_{t'}^{t'+T} I(V(t)) e^{-\kappa Z_n \cos(\omega t)} dt$$  \hspace{1cm} (B.1)

However, this approach faces implementation challenges in the final step, where spectroscopic noise is derived from current noise with a lock-in amplifier. A digital lock-in amplifier that replicates the STM lock-in amplifier is difficult to implement due to the restricted access to sample data. The STM’s lock-in amplifier is implemented within the STM’s FPGA and calculates LIY using the raw 1 MHz channel data.
B.2 Z-LIY Propagation

Figure B.2: Successful noise reduction in current signal. This uses the exact propagation from the geophone to the Z noise with a transfer function and then to the current noise with \( e^{-\kappa Z} \). However, the goal of spectroscopic noise cancellation is reducing noise in LIY and not current.

stream. In contrast, the Python script only has access to a 20 kHz data stream which is downsampled from the raw 1 MHz channel. In addition, the FPGA lock-in amplifier has access to the exact bias modulation reference signal whereas the Python script can only measure the bias modulation experimentally. These two factors inhibit an accurate replication of the STM’s lock-in amplifier output and introduced more error than any attainable noise reduction.

B.2 Z-LIY Propagation

To circumvent the implementation challenge of the lock-in amplifier, an approximation (outlined in Equation 2.8) assumes \( e^{-\kappa Z} \) to fluctuate at a low frequency relative to the lock-in frequency and brings the noise term outside the integral. This approximation reduces the need for the third step from the exact approach and directly applies the \( e^{-\kappa Z} \) noise term to the LIY signal. The results in Figure B.4 demonstrate an effective cancellation of positive noise but the negative noise is essentially unchanged. A conjecture for this asymmetric behavior is the approximation neglects...
Figure B.3: The Z-LIY propagation does not effectively reduce negative noise. By approximating the noise as constant across a modulation period, the LIY can be treated similarly to the current signal in Figure B.2. However, an asymmetric noise reduction is visible between the measured and processed data and this phenomenon is not fully understood.

the combined effect of aliasing in the lock-in amplifier and the asymmetric effect of exponentiation of the noise. When carrying the noise term out of the integral, only the principal frequency of the noise $\omega_n$ is considered. However, the lock-in amplifier reproduces the noise at $\omega_n, \omega \pm \omega_n, 2\omega \pm \omega_n, \ldots$. In addition, negative current noise is more pronounced compared to positive current noise as the noise is proportional to $e^{-\kappa Z}$. The neglected higher frequency noise combined with the exponential relationship causes larger negative noise than detected on the geophone, leading to the asymmetric noise reduction behavior.

B.3 G-LIY Direct

In this approach, the additional approximation using the Taylor expansion of $e^x$ means a transfer function can be directly calibrated between Z and LIY. The subsequent application and results are discussed in Section 2.1.2 and Figure 4.4 is reproduced below. The asymmetric behavior is not apparent in this approach as the transfer function was calibrated on similar data and likely incorporated the greater negative noise in the phase and amplitude information at each frequency.
Figure B.4: The G-LIY approach successfully attenuates both positive and negative noise values. The processed LIY signal significantly reduces vibrational noise, despite changes in the vibration amplitude over time. The noise reduction is significantly greater than the other three approaches.

Figure B.5: The G-log(LIY) approach performs worse than the G-LIY approach. The ineffective negative noise reduction behavior is similar to the behavior found in Figure B.4. The results are contrary to the intended results, as calibrating on log(LIY) rather than LIY is meant to account for the exponential behavior between the geophone and current signal.
B.4 G-log(LIY) Direct

This approach was meant to be an evolution on the G-LIY direct approach; a transfer function is calibrated between G and log(LIY) to eliminate the need for the Taylor expansion approximation. By taking the log of LIY, the exponential relationship of $e^{-\kappa Z}$ is reduced to a linear effect in log(LIY) for an accurate calibration between G and log(LIY). The application of the transfer function is slightly more involved (Equation B.2) than the direct approach, but relatively easy to implement compared to the first two approaches. Despite the intention of this approach to further reduce noise compared to the G-LIY direct approach, the results in Figure B.5 actually show a poorer performance in reducing negative noise than the previous approach. It is likely the same effect as conjectured in Section B.2 exists here and the transfer function could not capture the negative noise as well as the transfer function in the previous approach.

$$LIY_s \approx \exp \left[ \log(LIY_m) - \left( \tilde{G}T_{\log(LIY)} \right)^{-1} \right] \quad \text{(B.2)}$$

Conclusion

G-LIY direct is the most effective approach towards reducing spectroscopic vibrational noise. In both the Z-LIY propagation and G-log(LIY) direct approaches, the scheme successfully reduced positive noise but was ineffective in attenuating negative noise. Although the exact propagation approach does not require any approximations, the challenges of a lock-in amplifier hinder the implementation of this approach. Therefore, G-LIY direct represents the best approach for this thesis, although future work could resolve the implementation challenges of an exact propagation approach.
Appendix C

Budget
BOM (Bill of Materials) Unit Cost $ Unit # of Units Total $ Exact or estimated?

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If you had to use CNS space and equipment please answer the following:

Why did your project require the use of CNS facilities?

What is the minimum cost to make one prototype of your project ($0 is an option)?

Roughly much time did you spend using CNS facilities [specify hours or days]?

What equipment did you need to use?

Total cost covered by the Harvard Research Lab(s) you are affiliated with, if any

Total cost covered by a non-Harvard lab, if any

Please list below all material used in ALL that were not accounted for in your budget

What could we have done better to make your CNS experience more productive?

Please list below all material used in ALL
References


