We promote the use of Python through the Anaconda open data science platform. We are aware that other installation methods exist, but have solely included the Anaconda installation instructions below due to the ease of setup and use in a classroom environment:

**Installation Instructions for Windows Users**

1. In order to download Anaconda for Windows, navigate to the following webpage: <https://www.anaconda.com/download/>
2. In the section labeled “Anaconda for Windows”, there are installers for Python 2.7 and Python 3.7. The Schrodinger.py program is written for Python 2.7 and 3.7. *While you may want to install both versions of Python for personal use, the following instructions are provided for version 3.7 only.*
3. In the box labeled “Python 3.7”, click on the blue box labeled “WINDOWS 64-BIT GRAPHICAL INSTALLER.” *If you are using Windows 32-bit, the graphical installer is provided in smaller print below the 64-bit installer.*
4. Upon clicking the installer, you will notice a dialog box appear at the bottom of your web browser, indicating the download progress. Once finished, click the executable to begin the installation. If a dialog box does not appear, navigate to the Downloads folder from the desktop or windows key, and double click the executable to begin installation.
5. Upon double clicking the executable, the Anaconda 64-bit Setup Wizard will open. Click “Next” to continue.
6. Click “I Agree” to accept the license agreement.
7. Select “Just Me” as the installation type. This will complete the installation without requiring administrative privileges.
8. Next, you will be prompted to select an installation location. Here, it is most likely that the default location is suitable. For example, the destination folder that we selected was **C:\Users\Username\Anaconda3** where Username is your name.
9. You will then be prompted for two installation options (add Anaconda to my PATH environment variable and Register Anaconda as my default Python 3.7). We advise that both these boxes are checked before proceeding.
10. Click “Install”. The installation process will take some time, please be patient.
11. Upon installation, several executables are generated. In order to find these executables, open Windows’ File Explorer and navigate to the installation location directory you specified in step 8 above. Upon locating this “Anaconda3” folder, you will find a subfolder called “Menu”. This folder contains all the executables that you will utilize for running Python programs or Jupyter notebooks. We advise copying the important executables as shortcuts to your desktop so that they are easier to access. The executables you will use most frequently are: Jupyter, Jupyter Notebook, Anaconda Prompt, and Spyder.
12. Once you have created shortcuts for the above executables, open the Anaconda Prompt. Upon opening, the prompt will appear similar to Windows Command Prompt. You will notice the path of your installation location from step 8 to the left of the Anaconda Prompt, followed by a cursor.
13. In the Anaconda prompt, type **conda update conda**.
14. A list of packages to be downloaded will appear and you will be asked to proceed [yes/no]. Select yes to begin the download.
15. Following the download, you will also need to manually install the numpy, scipy, matplotlib, and colorama packages. In order to install each of these, use the following example for formatting purposes: **conda install numpy.** After typing each install command once, type the same command a second time to assure that the package is correctly installed. If installed, you will receive the following message upon typing the install command a second time: “All requested packages already installed.”
16. We also advise that you create a folder on your desktop called **myJupyterProjects**.
17. Next, open an Anaconda Prompt and navigate to the myJupyterProjects desktop folder that you just created in step 16. In order to navigate directories using the Anaconda Prompt, the following Windows Command Prompt keystrokes should be utilized:

* **dir** = list files in your current directory
* **cd** = change directory (in order to use the **cd** command, you must first type **cd** followed by a **space**, followed by the **name** of the folder or directory you wish to navigate to)
* **cd ..** = move back one folder level

As an example, when you open your Anaconda Prompt, the default folder should be identical to what you declared in step 8 above (**C:\Users\Username\Anaconda3)**. If this is the case, you will simply type **cd Desktop\myJupyterProjects** to navigate to the myJupyterProjects folder on the desktop that you created in step 16.

1. Once you’ve navigated to the myJupyterProject folder via the Anaconda Prompt, type **jupyter notebook** in the Anaconda Prompt. This will open jupyter in your default web browser.
2. With the notebook open, users are encouraged to examine the options at the top of the web browser. Most importantly, the user should focus on the “play” button in the top panel, which can be used to run each cell in the Jupyter notebook. The Jupyter notebooks are broken down into sections of **markdown** (text that explains the Schrodinger program or theory/math behind the program) and **code** (Python commands that carry out the mathematics discussed in the manuscript). When using the notebook, users should progress through the cells of the notebook one-by-one and press the play button for each cell. This will update the screen of any changes and also prompt the user for any input that the program requires. In the edit tab of the top panel, users also have the option to **run all cells**. If the user updates markdown text or Python code, they must remember to press the play button to update the screen of those changes. In some instances, the user might need to begin at the beginning of the notebook and re-play all the cells again, or simply use the **run all cells** function.
3. When finished, the Jupyter notebook should be closed. However, the main jupyter web browser will remain open and the Jupyter notebook will show **Running** in green. Click on the green **Running** and an option will appear to **Shutdown** the notebook. Click **Shutdown** before closing the main jupyter notebook web browser. Last, press CTRL+C in the Anaconda Prompt to terminate the juptyer notebook process.

**Links for Getting Started with Markdown**

<https://jupyter-notebook.readthedocs.io/en/stable/examples/Notebook/Working%20With%20Markdown%20Cells.html>