

QuantumWell

Python-based time-independent Schrodinger equation solver using PyQt5 to specify and view a variety of quantum wells, including wells with multiple barriers. The user specifies well parameters or accepts default values. No knowledge of python is necessary. Grinnell College students have used this project since 2016 in their modern physics courses. It was last tested with anaconda python 3.6/7/8, October 2020, for Windows 7 and 10, macOS Catalina, and Linux.

Getting Started

This package uses python3 and a variety of python modules. If you are new to python, it's easiest to install a python platform such as the widely used [anaconda individual edition](#). We are currently using anaconda with python 3.8 installed with the anaconda graphical installer using these [installation instructions](#).

Prerequisites

- macOS, Windows 7/10, or Linux operating system
- python > 3.5, DO NOT USE PYTHON 2.x
- python modules numpy, scipy, pyqt (version 5), matplotlib, and their prerequisites; all are included in the anaconda platform.

Unless you use additional python platforms, I recommend that users new to python take the anaconda install defaults while paying particular attention to these two options:

1. Select *Install for me only* rather than selecting *Install for all users* to avoid needing admin privileges.
2. For installs on Windows, select *Add Anaconda3 to my path environmental variable* even though the installer recommends not using this option. Otherwise, you will have path issues when using the QuantumWell startup scripts.

Installing and Opening the main GUI

- Download the compressed file from Github by double-clicking <https://github.com/dukeclid/QuantumWell/archive/main.zip>.
- Move the downloaded file to any directory; I recommend your Desktop. If necessary, decompress and extract the contents (double-clicking usually works). You should see the QuantumWell-main directory.
- (OR if you are familiar with git software, you may obtain a clone of the git repository. The main directory name will now be QuantumWell. The -main from the zipped file shows that the downloaded file is the contents of the main branch in the repository.)
- From now on, I will use the name, QuantumWell, for the QuantumWell-main directory.
- Open a file browser in the QuantumWell directory. Execute the config script by double-clicking on:

- `config.bat` for Windows
- `config.command` for macOS
- `config.sh` for Linux os.
- or from a terminal window in the QuantumWell directory, execute `python config.py`

The `config.py` script first determines if you have all the QuantumWell prerequisites. It then proceeds to create a startup script for the GUI and records the path to the QuantumWell directory in a config file.

Depending on your operating system, the `config.py` script produces one of the following startup scripts both in your QuantumWell directory and on your Desktop:

- `startQWell.bat` script for Windows machines
- `startQWell.command` for macOS machines
- `startQWell.sh` script for Linux systems

You can copy the appropriate `startQWell.xx` to any directory you wish and open the GUI from there.

The `config.py` python script also creates a `qwconfig/config` file off of your home directory which contains the path to your QuantumWell directory and can be used to set the path for importing modules from the `src` directory into e.g. jupyter notebooks. There are more details in the [Documentation/UsersGuide](#). If you are only using the GUIs, you can ignore this paragraph.

Open the QuantumWell GUI by

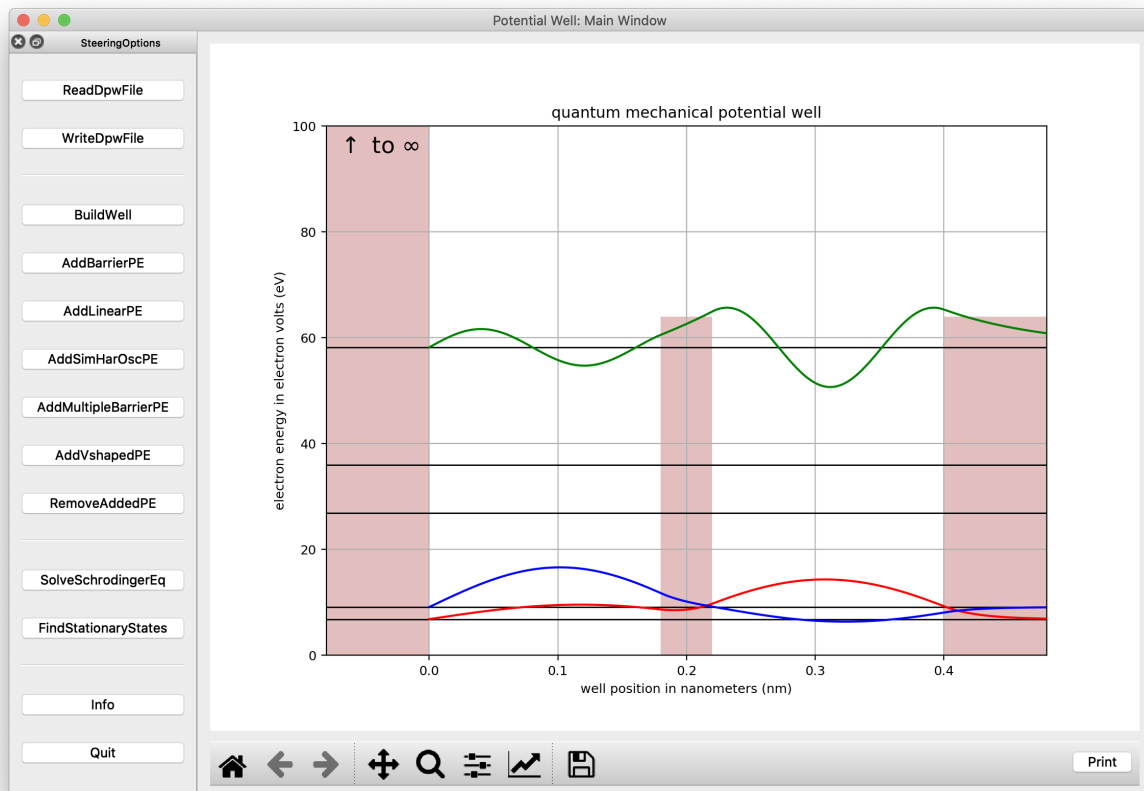
- Double-clicking the `startQWell` script from a file browser set on any directory containing the script.
- or from a cmd Windows terminal typing,
`python <path to QuantumWell directory>\quantumWell.py .`
- or from a macOS or Linux terminal typing,
`python <path to QuantumWell directory>/quantumWell.py .`
- or open a terminal, `cd` to the location of your `startQWell` script, and execute the script from the terminal prompt.

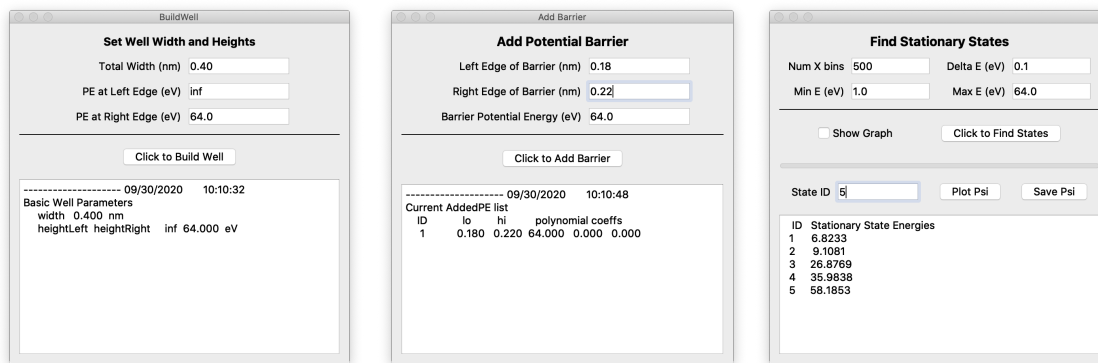
Usage

The QuantumWell GUIs are largely selfexplanatory. Each button on the main GUI opens a side window to set and record well parameters. The *SolveSchrodingerEq* window shows the wavefunction for a given energy (and will diverge if the energy is not a stationary-state energy). The *FindStationaryStates* window permits determination of the stationary-state energies and plotting selected state wavefunctions on the main window. The always present *Message* window shows the history of your session; sending the history to a file and/or to a printer are *Message* window options.

You can find more details in the [Documentation/UsersGuide](#)

Here is an image of the main window after using default parameters from the *BuildWell*, *AddBarrierPE*, and *FindStationaryStates* windows. Images of these windows follow the main window.





Tutorials

The `Tutorials` directory contains jupyter notebook tutorials to provide guides for using the QuantumWell modules in user constructed jupyter notebooks. There is more information about these modules in the [Documentation/UsersGuide](#)

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