latticegraph$_{d}esigner Documentation$

Release latest

May 15, 2017

Contents

CHAPTER 1

NOTE: Documentation is curently in development!!!

Lattice graph designer 1.0a1

Lattice graph designer is a tool which allows to visualize and create a lattice graph model using the intuitive GUI and interactive 3D drag-and-drop graph manipulation pane. It was primarily created for the ALPS project to deal with a lattice graph of the Heisenberg model defined in ALPS xml graph format. Support of the other formats and projects can be extended.

- Git-hub repo: https://github.com/luchko/latticegraph_designer
- Documentation: https://latticegraph-designer.readthedocs.io
- Free software: MIT license

GUI is based on PyQt. Program is compatible with Python 2.7 or Python 3.3+ and PyQt4 4.6+ or PyQt5 5.2+.

Features

- import and visualisation of the lattice graph saved in the ALPS compatible lattice graph xml format.
- import the crystal structure providing the unit cell parameters, sites coordinates and the space group symmetry operations.
- import the crystal structure from the CIF file.
- export the lattice graph to the ALPS compatible xml file.
- interactive 3D drag-and-drop graph manipulation pane based on matplotlib
- manipulation edges (add, remove, change type) referring to the distance between vertices they connect.

- xml code editor (highlighting, synchronization with manipulation pane)
- exporting the figure of the lattice graph model.
- animation manager allows to animate a 3D model and save the animation in mp4 or gif format.
- preferences manager allows setting the visual theme of the lattice graph displayed on the manipulation pane.

Dependencies

- **Python** 2.7 or 3.3+
- **PyQt4** 4.6+ or **PyQt5** 5.2+ : PyQt4 is recommended.
- **NumPy**
- **Matplotlib**

Important note: *Most dependencies listed above are installed automatically, however in some cases you might need to istall them separately (see next section).*

Install PyQt4 or PyQt5

- in case you use conda type: `$ conda install pyqt=4` (or 5)
- otherwise follow the links PyQt4 or PyQt5.

Install all other dependencies

```
$ pip install -r requirements.txt
```

or, incase you use `conda`

```
$ conda install --file requirements.txt
```

Installation and launching

This section explains how to install and launch the latest stable release of the Lattice graph designer in one of the cross-platform ways listed bellow. If you prefer testing the development version, please use the bootstrap script (see next section).

Installation using `conda` scientific package manager (recommended way)

PROJECT IS NOT RELEASED YET

Type in your command prompt:

`$ pip install conda` (if `conda` is not installed yet)

```
$ conda install latticegraph_designer
```

Note: *All dependencies are installed by* `conda` *automatically.*

Installation using `pip` package manager from PyPI

PROJECT IS NOT RELEASED YET

Type in your command prompt:

```
$ pip install latticegraph_designer
```

Important note: *This also installs all dependencies except PyQt4 or PyQt5. Those have to be installed separately after installing Python.*

Installation from source

Note: *This is temporary installation way untill the using of* `conda` *or* `pip` *is not implemented.*

- Download a source of the last stable package version.
- Open the terminal and move to the package root directory.
- In your command prompt type:

```
$ python setup.py install
```

Launching the program

- After completing the installation you can launch the program simply typping in your command prompt:

```
$ graphdesigner [pathToYourLatticeGraphFile.xml]
```

note If `pathToYourLatticeGraphFile.xml` is not provided the program will load a default example. You can open a lattice graph file later.

- Optionally you can lock a tool's link on the launcher for quick access.

Running from source

The fastest way to run LatticeGraph designer is to follow this steps:

1. Make sure that all dependencies are installed.
2. Download a source of the last stable package version.
3. Run `$ python bootstrap.py` from the package root directory.

You may want to do this for fixing bugs, adding the new features, learning how the tool works or just getting a taste of it.

Running `unittest`

After making any changes in the source code you can run `unitittest` to make sure that nothing is broken by typing in your command prompt:

```
$ python setup.py test
```

Note: *In case ALPS library is installed* `unitittest` *also checks for ALPS compatibility of the exported xml lib file using ALPS* `printgraph` *tool.*

Contacts

About the feature extension or bugs report you can create the issue or feature request or feel free to contact me directly by e-mail:

Ivan Luchko - luchko.ivan@gmail.com

Widgets references

- Matplotlib animation manager
- QCodeEditor

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CHAPTER 2

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```
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Note: *All dependencies are installed by* `conda` *automatically.*

Installation using `pip` package manager from PyPI

PROJECT IS NOT RELEASED YET

Type in your command prompt:

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