

qd

qd is a simple, pedagogical implementation of TDDFT for 2D systems.
for qd Version 0.1.0

by The 2014 Benasque TDDFT School

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Version 3, 29 June 2007

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2 Overview

The GNU `qd` program is a simple, pedagogical implementation of TDDFT for 2D systems. It is a very primitive program, thought as a platform for learning and experimenting on the theory. Because it is protected by the GNU General Public License, users are free to share and change it.

GNU `qd` was written by The 2014 Benasque TDDFT School.

3 Sample Output

This is the output of the command ‘qd’:

```
qd 0.1.0
Written by The 2014 Benasque TDDFT School.
```

```
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```

As you can see, a useless greeting. Here is the output of the command ‘qd --help’:

```
Usage: qd [OPTION...]
qd is a simple, pedagogical implementation of TDDFT for 2D systems.

-c, --coefficients      Generates coefficients for the discretization
-e, --test_exponential  Tests the exponential
-g, --gs                Performs a ground state calculation
-h, --test_hartree      Tests the Poisson solver
-l, --test_laplacian    Tests the Laplacian
-s, --strength_function Calculates the strength function
-t, --td                Performs a time-dependent calculation
-x, --excitations       Performs a LR-TDDFT calculation
-?, --help              Give this help list
    --usage              Give a short usage message
-V, --version            Print program version
```

Report bugs to acastro@bifi.es

4 Invoking qd

The format for running the qd program is:

`qd option ...`

qd supports the following options:

- `--help`
- `-?` Gives a help list
- `--usage` Gives a short usage message
- `--version`
- `-V` Print the version number of qd on the standard output and then exit successfully.
- `--coefficients`
- `-c` Generates coefficients for the discretization
- `--test_exponential`
- `-e` Tests the exponential
- `--gsn`
- `-g` Performs a ground state calculation
- `--test_hartree`
- `-h` Tests the Poisson solver
- `--test_laplacian`
- `-l` Tests the Laplacian
- `--strength_function`
- `-s` Calculates the strength function
- `--strength_function`
- `-s` Calculates the strength function
- `--td`
- `-t` Performs a time-dependent calculation
- `--excitations`
- `-x` Performs a LR-TDDFT calculation

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