Spectrum Calculator for the Krugler-Montgomery-McConnell Hamiltonian

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Installation

These installation instructions are for machines running UNIX/Linux with the Bash shell.

Option I: Getting the executables

1) Download the archive "KMMexec.zip" to any empty directory and unpack it.
2) Go to that directory in the *Terminal* and run the installation script `srcexec` (type `sh srcexec` in the command line).

Option II: Compiling the source code yourself

Note: this option requires that you have the GNU Compiler Collection (gcc) installed!

1) Download the archive "KMM.zip" to any empty directory and unpack it.
2) Go to that directory in the *Terminal* and run the installation script `srccomp` (type `sh srccomp` in the command line).

For both options:

The package is installed in `$HOME/Applications/KMM`. To run it, you will need to add this destination to the PATH environmental variable. To do this, go to your home directory (`cd $HOME`), open or create the file `.bash_profile`, and add the following lines:

```
PATH=$PATH:$HOME/Applications/KMM
export PATH
```

Close and source the file (`source .bash_profile`) or restart your computer.
The program is ready to run!

Running the program

The program can be launched from the terminal using the `kmm` command, followed by the input file name:

`kmm` *`file`*

Input file

The input file contains three parameters: 1) the size of the system; 2) the coupling (in units of ε); 3) the switch for turning on and off analysis of the 4-excitation manifold. The parameters must be in this order. A sample file looks as follows:

```
Number of sites: 50
Coupling (in units of epsilon): -0.51
Analyze 4-excitation manifold: yes
```

The text before the colon is an optional comment that can be modified or omitted altogether. The colon itself, however, must be included:

This input file will work	This input file will NOT work

`: 50`
`: -0.51`
`: yes`
	`50`
	`-0.51`
	`yes`

Sample input files `Sample_strong` and `Sample_weak` are included in the installation package. The number of sites should be an even number ≥ 4. The coupling can be any negative number, except those in the range $0.499999 < |b| < 0.500001$, restricted to avoid divergence at the critical point $|b| = 0.5$. The program will accept the options *yes (Yes, y, Y)* and *no (No, n, N)* for the third parameter. *Please note that switching on the analysis of the 4-excitation manifold slows the calculation down considerably*. For a system of 100 sites, the calculation may take under a minute when the third parameter is set to *no*, and 5–10 minutes or more when it is set to *yes*. For a system of 200 sites, analysis of the 4-excitation manifold can be expected to take several hours.

Output files

*n*FinIntens.out

This file is written separately for each n-excitation manifold analyzed: thus, in the weak coupling regime, $2|b| < \varepsilon$, $n = 1$ and 3, while in the strong coupling regime, $2|b| > \varepsilon$, $n = 2$ and 4 (if analysis for the 4-excitation manifold is turned on). The file contains three columns: 1) The excitation energy of a state; 2) the total k-vector of a state; 3) the matrix element squared for the excitation to the given final state from the ground state. *For large system sizes and higher excitation manifolds this file can be very large (several GB)!*

Overlap.out

This file is only written for the strong coupling regime, $2|b| > \varepsilon$. It contains a single number: the matrix element squared for excitation from the ground state $|\Phi_+\rangle$ to the lowest excited state $|\Phi_-\rangle$. The energies of these two states can be found in the program output that is written to the screen. Look for the following lines:

```
Minus vac. = -X.XXXXXXXXXXXXXXXXXXX
Plus vac.  = -X.XXXXXXXXXXXXXXXXXXX
```

For larger system sizes, the energy difference between these states is very close to zero.

ZGrid_*n*exc.out

This file contains the linear absorption density written in grid format on a rectangular grid. The wavenumber range is [–10/a; +10/a], with 640 grid points. The energy range is [0, 6ε], with 480 grid points. The file is formatted for plotting with Gnuplot using the included script. One file is written for each n-excitation manifold analyzed.

EkIrange.out

This file contains the minimum and maximum wavenumber, energy, and excitation intensity for each excitation manifold analyzed.

Plotting the output with Gnuplot

The files `ZGrid_nexc.out` contain grid data that can be plotted using the Gnuplot "with image" option:

```
plot 'ZGrid_nexc.out' w image
```

Using a high-contrast color map, such as RGB (8, 15, 36), will show more details of the spectrum:

```
set palette rgbformulae 8, 15, 36
```

It is also possible to create 3D plots of individual transition intensities from the files `nFinIntens.out`:

```
splot 'nFinIntens.out' w imp
```

This is most useful for $n = 1$, since in the 1-excitation manifold there are only as many transitions as there are sites, so individual transitions are clearly distinguishable. *Do not attempt this for very large files (e.g., `nFinIntens.out` for higher excitation manifolds).*

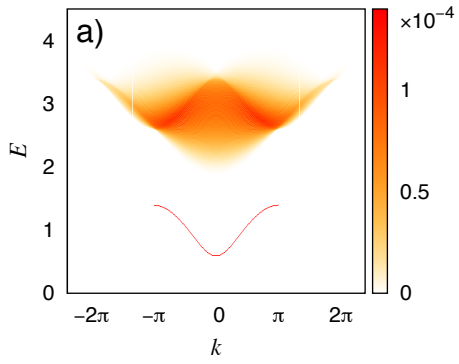
For details of the model refer to: A.A. Kocherzhenko, J. Dawlaty, B.P. Abolins, F. Herrera, D.B. Abraham, K.B. Whaley. *Collective Effects in Linear Spectroscopy of Dipole-Coupled Molecular Arrays.*

Appendix: Sample Gnuplot script

Here is a sample Gnuplot script:

```
set term postscript enhanced eps color "Helvetica" 16 size 2.30, 1.97
set palette rgbformulae -2, -3, -6
set xrange [-7.5:7.5]
set xtics ('{/Symbol -}2{/Symbol p}' -2*pi, '{/Symbol -p}' -pi, 0,
          '{/Symbol p}' pi, '2{/Symbol p}' 2*pi) scale 0
set yrange [0:4.5]
set ytics 0, 1 scale 0
set cbrange [0:1.4e-4]
set cbtics ('0' 0, '0.5' 5e-5, '1' 1e-4,
           '{/Symbol {\264}}10^{{/Symbol -}4}' 1.35e-4) scale 0
set xlabel "k" font "Times-Italic, 18"
set ylabel "E" offset 1 font "Times-Italic, 18"
unset label
set label "a)" at graph 0.03,0.92 front font "Helvetica, 24"
set output "filename.eps"
plot 'datafile1.out' w image notitle, 'datafile2.out' w image notitle
```

This is the output it produces:



You will need to adjust `cbrange` and `cbtics` for your specific data set.