XMGRACE INFO

The data files in this repository are stored as .xmgrace files. Grace is a free WYSIWYG 2D graph plotting tool, for Unix-like operating systems. You can find more info on <https://en.wikipedia.org/wiki/Grace_(plotting_tool)>.

To execute .xmgrace file, you simply need to run this command on any Unix-like operating system:

***xmgrace file.xmgrace***

The data associated with our work, “Density matrix superoperator for periodic quantum systems and its application to quantum cascade laser structures” is stored in this format due to its compactness and an interested reader can reproduce any figure in our paper, with ease.

.xmgrace file is an ordinary text file and it can be open with any text editor. We advise Notepad++. The first set of lines has a form:

# Grace project file

#

@version 50123

@page size 792, 612

@page scroll 5%

@page inout 5%

@link page off

@map font 0 to "Times-Roman", "Times-Roman"

@map font 1 to "Times-Italic", "Times-Italic"

@map font 2 to "Times-Bold", "Times-Bold"

@map font 3 to "Times-BoldItalic", "Times-BoldItalic"

@map font 4 to "Helvetica", "Helvetica"

@map font 5 to "Helvetica-Oblique", "Helvetica-Oblique"

@map font 6 to "Helvetica-Bold", "Helvetica-Bold"

@map font 7 to "Helvetica-BoldOblique", "Helvetica-BoldOblique"

@map font 8 to "Courier", "Courier"

@map font 9 to "Courier-Oblique", "Courier-Oblique"

@map font 10 to "Courier-Bold", "Courier-Bold"

@map font 11 to "Courier-BoldOblique", "Courier-BoldOblique"

@map font 12 to "Symbol", "Symbol"

@map font 13 to "ZapfDingbats", "ZapfDingbats"

Lines starting with “@” are instruction for Grace plotting tool. The lines can be easily understood as simple figure settings, they set up x-y limits, colors, legends etc. What is important to understand in this file is how data information is stored.

Every graph in a figure has a label G0, G1, G2 … etc, every trace on a given graph has a label S0, S1, S2 … etc. For a standard x-y plot, only 1 graph and 1 trace exist, and info is stored after the line starting as @G0.S0, if the plot has multiple traces, next one will be at @G0.S1 etc.

If the figure has insets or different y-axis scaling (L-I-V figure for example), the first graph and its traces would be labeled as G0.S0, G0.S1, G0.S2 … etc, and the inset data would be stored in G1.S0, G1.S1, G1.S2 … etc.

In this repository, we stored the figure names in format Figure\_X\_number.xmgrace. X is the figure of interest, while number is the line in .xmgrace file where first trace in figure begins (after the command @target G0.S0). Note that xmgrace files pack all the x-y points after the instructions for the grace plotting tool, and you can find all the data after the first occurrence of G0.S0 or simply use ctrl+F and find a line starting having G0.S0 or any Graph.Trace you are interested in.

For a non-Unix user, we recommend following steps of retrieving the data from our figures:

1. You can freely delete first “number” lines in Figure\_X\_number.xmgrace, from that point you will have the data for every graph and every trace in the Figure\_X.
2. To find specific trace, you can navigate through the .xmgrace file with ctrl+F searching for specific graph.trace in form Gi.Sj, where i and j are indices of interest.
3. For your convenience below is a table of all the traces for each figure individually:

|  |  |  |  |
| --- | --- | --- | --- |
| Figure name | Graph | Trace | Description |
| Figure\_2\_629.xmgrace | G0 | S0 | at (blue) |
| S1 | at (red) |
| G1 | S0 | at (blue - inset) |
| S1 | at (red - inset) |
| Figure\_3\_443.xmgrace | G0 | S0 | Band structure potential (black) |
| S1 | Ground state wavefunction (red) |
| S2 | The second state wavefunction (green) |
| S3 | The third state wavefunction (blue) |
| Figure\_4\_346.xmgrace | G0 | S0 | for pentadiagonal model (bluel) |
| S1 | for tridiagonal model (red) |
| Figure\_5\_1295.xmgrace | G0 | S0 | at (black) |
| S1 | at (red) |
| S2 | at (green) |
| S3 | at (blue) |
| S4 | at (cyan) |
| S5 | at 5e5 (purple) |
| G1 | S6 | at (black - inset) for the nearest neighbor approximation |
| S7 | at (red - inset) for the nearest neighbor approximation |
| S8 | at (green - inset) for the nearest neighbor approximation |
| S9 | at (blue - inset) for the nearest neighbor approximation |
| S10 | at (cyan - inset) for the nearest neighbor approximation |
| S11 | at 5e5 (purple - inset) for the nearest neighbor approximation |
| S12 | at (dashed black - inset) for the second nearest neighbor approximation |
| S13 | at (dashed red - inset) for the second nearest neighbor approximation |
| S14 | at (dashed green - inset) for the second nearest neighbor approximation |
| S15 | at (dashed blue - inset) for the second nearest neighbor approximation |
| S16 | at (dashed cyan - inset) |
| S17 | at 5e5 (dashed purple - inset) for the second nearest neighbor approximation |
| Figure\_6\_597.xmgrace | G0 | S0 | for tridiagonal model (black) |
| S1 | for pentadiagonal model (red) |
| G1 | S0 | for tridiagonal model (black – inset) |
| S1 | for pentadiagonal model (red – inset) |

We apologize to the interested reader for the unorthodox storage of the data, but keep in mind that if we provided every individual x-y trace in a separate file, the repository would consist of very large number of files that would be hard to process. In this way, readers with access to Unix-like system can reproduce are figures with ease, while a Windows user would need to open the Figure\_X\_number.xmgrace files, ignore first “number” of lines in it and navigate to the trace of interest with the help of the table above.

\*Note that in figure 5 the notation is slightly difference and first trace is G0.S6 instead G0.S0.

Kind regards,

The authors