User Guide of FROG

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Abstract

This Guide provides you information on how to install the FROG program to your PC, calculate the DOS and linear response functions and visualize the output.

1 Introduction

FROG (**F**requency dependent **R**esp**O**nse function **G**enerator) is a group of programs based on the *Projection Method* [1] for calculating linear respose function with amazing efficiency. This method is can be and has been applied to nanosctructres [2], Anderson localization models [3] and quantum spin systems at finite temperatures [4]. The executable program contained in this package is a paticular version developped for calculation of quantum spin systems on WindowsXP machine.In the future, programs for other problems on other machines will be included in this package as a united program and/or a group of sister programs.

2 What problems does it solve?

The quantum spin system FROG takes care of is described by the Hamiltonian,

$$H = \sum_{<i,j>} J_{ij}\vec{S}_i \cdot \vec{S}_j + \sum_{<i,j>} \vec{D}_{ij} \cdot \left(\vec{S}_i \times \vec{S}_j\right) - g\mu_B \vec{H} \sum_i \vec{S}_i. \tag{1}$$

where J_{ij} is exchange interaction, D_{ij} is Dzyaloshinskii-Moriya interaction, and $\vec{H}$ is the external magnetic field.

2.1 linear response function

First, FROG computes the correlation function in time domain,

$$g_q^\mu(t) = \mathrm{Tr}\left[e^{-\beta H} M_{-q}^\mu e^{+iHt} M_{+q}^\mu e^{-iHt}\right] / \mathrm{Tr}\left[e^{-\beta H}\right] \tag{2}$$

where $\beta = 1/(k_B T)$ is inverse temperature and $M_q^\mu = \sum_{j=1}^{N_{spin}} s_j^\mu \frac{e^{iqj}}{\sqrt{N_{spin}}}$ is the magnetization operator. Then FROG calculates the dynamical magnetic

susceptibility $\chi_{\mu\mu}(q,\omega)$ by Fourier transformation,

$$\chi\mu\mu(q,\omega) = (1 - e^{-\beta\omega}) \lim_{\eta \to +0} \int_0^\infty dt e^{-i(\omega - i\eta)t} g_q^\mu(t) \tag{3}$$

3 Terms of Use

- This package is provided for free trial use of FROG during the given period. It can be distributed freely as a whole package (i.e. as a FROG??.zip file).
- The copyright of this package belongs to Toshiaki IITAKA.
- We do not have any responsibilities for possible damages caused by the use of this package.

4 System Requirements

- PC with WindowsXP. FROG may run ohter versions of Windows, but not confirmed.)
- wgnuplot, Windows version of gnuplot. Available at
  ftp://ftp.gnuplot.info/pub/gnuplot/gp400win32.zip
  This is our standard visualizer for FROG, but it is optional. Your favourate graph plotting program can be used for visualizing the ascii output data.

5 Install

- Unzip the FROG???.zip file. You will find in the folder the executable file 'frog.exe', and example input files 'ex??.in'.
- Copy this folder wherever you like.

6 Run FROG

- Open a *command window* of WindowsXP from the folder. Execute the FROG with a input file.

  ```
  >frog.exe < ex1.in
  ```

  The FROG will generate three ascii output files in the folder.

  - **gij**: correlation function in time domain.
  - **dos/chi**: DOS or linear response function in energy domain.
  - **gnu.plt**: command file for gnuplot. You can load this file from gnuplot to visualize gij and dos/chi files. You may edit this file to obtain a prefered look and feel of the graph. If you do not use gnuplot, you can visualize the ascii files by using your plotting program directly.

References

[1] T. Iitaka, S. Nomura, H. Hirayama, XW. Zhao, Y. Aoyagi, T. Sugano, Calculating the linear response functions of noninteracting electrons with a time-dependent Schrodinger equation, Phys. Rev. E 56, 1222-1229 (1997).

[2] S. Nomura, T. Iitaka, XW. Zhao, T. Sugano, Y. Aoyagi, Linear scaling calculation for optical-absorption spectra of large hydrogenated silicon nanocrystallites, Phys. Rev. B 56, R4348-R4350 (1997).

[3] T. Iiitaka, Fast Algorithm for Quantum Physics, RIKEN Review No.19, 136-143 (1998).

[4] T. Iitaka, T. Ebisuzaki, Algorithm for linear response functions at finite temperatures, Application to ESR spectrum of s=1/2 antiferromagnet Cu benzoate. Phys. Rev. Lett. 90, 047203 (2003).