

Update of GnXAS package

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Abstract

Several Fortran programs of the GnXAS package have been revised and upgraded in the last two years by C. R. Natoli, A. Filipponi and A. Di Cicco. The phase-shift generation program (phagen) is now able to calculate phase shift using accurate relativistic corrections. Output phase-shift files contain the result of the calculations using different approximations. The gnXAS program has been updated mainly to overcome some old-fashioned limitations of the output for data (ASCII multicolumn files for the derivatives) and graphics (gnuplot in place of TopDrawer). Higher precision values of the fundamental constants were included both in gnXAS and fitheo programs. Variables were converted to double-precision in the fitheo minimization routine avoiding some precision issues observed in earlier versions. An extensive improvement of the fitheo output was carried out and now multicolumn data files and full gnuplot graphic output is available (on-screen and on selected formats) for multi-edge refinements. Programs have been tested in Camerino using Linux operative systems (Mint 19.3). This update should be used in addition to the current GnXAS handbook [1].

program phagen

The program has been extensively revised by C. R. Natoli and tested in Camerino, 2019. Major upgrades to the original GnXAS distribution [1,2] include:

- implementation of the relativistic corrections in the calculation of the phase shifts for the GnXAS suite of programs. See relevant papers [3], [4].
- new output files containing the `tl` scattering matrix. Calculations following the original non-relativistic scheme are produced with the same file extensions (`.tl`, `.s0` and so on). New calculations using the Dirac equation are with extensions: "nr" non relativistic, "sr" scalar relativistic, "so" spin-orbit relativistic (l+ and l-).

auxiliary program phaplo

A new `c` version `phaplo.c` (A. Filipponi 2021) has been developed.

This is an auxiliary program producing graphical visualization of the phase-shifts. The new version `phaplo.c` produces a multicolumn file and a color output for `gnuplot` (on-screen and `epslatex` script `.gnu`). The name extension are always `ABCpha.dat` and `ABCpha.gnu` so any calculation for different phases with the same `ABC` root filename will cancel the previous ones. Usage is similar to the original `phaplo` program, it just requires the input file name, for example:

```
phaplo.c ABCpha.sr (for scalar relativistic phase-shifts)
```

Real and imaginary part of the first phase shifts are visible (on-screen plot) for each prototypical atomic site. A `gnuplot` script `ABCpha.gnu` and the multicolumn file `ABCpha.dat` are also produced. The simple command

```
gnuplot ABCpha.gnu
```

produces `ABCpha.i.eps` high-quality postscript plots for `i=1,n` prototypical atoms.

program gnexas

An extensive revision was carried out by A. Filipponi in 2022. This includes:

- increased precision in the constants (`CF`, `PI`, `EV`) used for the MS calculations.
- introduction of new output for files containing derivatives: `.der` ASCII files. old output `.DER` binary files are retained in present version for continuity.
- generation of new multicolumn output data files for `G2`, `G3` and `GN` `.dat` containing the MS signals (first column `k(1/Ang.)`).

- production of new gnuplots epslatex source files G2n, G3 and GN .gnu producing high-quality graphic encapsulated postscript output (gnuplot GnABC.gnu -j GnABC.eps).
- on-screen on-the-fly display of undamped gamma(n) MS n-body signals (set presently x11 terminal, Linux).

program fitheo

New features of the program (A. Filipponi 2022, A. Di Cicco 2023).

Major upgrades of the fitting program made by A. F. include:

- conversion from single to double precision variables and functions avoiding mainly precision issues in the background refinement.
- updated values of the relevant constants of the calculations (slight changes in the k scales).
- reading of both .der (sequential-formatted) or .DER (direct-unformatted) MS derivative files.
- new single-edge on-screen graphical display (ptABC style) and multicolumn output for MS signals (mtABC.dat and mxABC.dat files).

Further upgrades (A.D.C.) include the extension to multi-edge cases and new and complete multicolumn and graphical output for gnuplot. This required extended coding efforts affecting input-output features of the program although it is presently compatible with older versions:

- graphical output: the IOUT card selects the types of graphical output as usual and described in the GNXAS documentation. For any choice IOUT=0-9 both Topdrawer and gnuplot output are produced, while when IOUT=10 (only gnuplot) can generate full output including runfit.par file. If IOUT \neq 4, as before, a second card is needed for compatibility (second IOUT=0-4 with different output features). For modern data-analysis the proliferation of files is not an issue anymore, so the suggestion is to use the IOUT=4 (second IOUT card) anyway.
- New output filename coding: .dat for multicolumn files and .gnu for gnuplot command files. New output filenames for TopDrawer: in this version pyABC.top (original filenames pyABC.dat), when Topdrawer output is selected. Output scr
- Multicolumn files containing the single-edge gamma n-body signals (mtABC.dat) and the individual MS signals (mxABC.dat) are produced also for multi-edge fitting for each edge under consideration 1..n (mt1, mt2, mx1, mx2... mxn).

- Multicolumn derADC.dat multi-edge files (derABC.dat single-edge, deiABC.dat, i=1,n for n edges) containing the derivative of the absorption spectrum (when selected) and some pre-analysis infos.
- Multicolumn noiABC.dat output with noise and expected residual estimate (with multiple file option, data appear ordered in energy).
- New psADC.gnu gnuplot script (epslatex) on noise evaluation and expected residual estimate. Gnuplot generates an encapsulated postscript high-quality figure (psABC.eps). The script can be edited to produce on-screen outputs or different formats.
- New paABC.gnu (single-edge) or paiABC.gnu, i=1,n (multi-edge) gnuplot script (epslatex) and on-screen gnuplot display on-the-fly of pre-analysis.
- New fgABC.dat and fxABC.dat multicolumn files containing the Fourier Transforms of total and individual MS signals (multi-edge fgiABC, fxiABC for i=1,n). Fourier Transform are calculated up to k=12 Ang-1.
- Multi-edge ptABC.gnu and pxABC.gnu gnuplot scripts (epslatex) showing the individual n-body signals (pt) and MS signals (px). Gnuplot generate encapsulated postscript high-quality figures (ptABC.eps and pxABC.eps). Scripts can be edited to produce on-screen outputs or different formats.
- Multi-edge fgABC.gnu and fxABC.gnu gnuplot scripts (epslatex) showing the Fourier Transforms of the individual n-body signals (fg) and MS signals (fx). Gnuplot generate encapsulated postscript high-quality figures (fgABC.eps and fxABC.eps). Scripts can be edited to produce on-screen outputs or different formats.
- Extension to multi-edge fitting of the on-screen on-the-fly graphical display of the individual n-body signals and total signals (only total signals are shown in multi-edge case in separate windows).

Other minor changes: increased dimensions for the number of data points (now 6000), elimination of reading binary data file and of several unused variables. Known bugs: problems in spline generation for the fixed JUMP selection (options CH2='J' and CH2='D') still not fully solved.

Bibliography

- 1] A. Di Cicco, A. Filipponi, Angela Trapananti, Emiliano Principi, Marco Minicucci, Agnieszka Witkowska, GNXAS. Extended suite of programs for advanced x-ray absorption data-analysis: methodology and practice., Editor A. Di Cicco, TASK publishing July 2009, ISBN 978-83-908112-8-4.
- 2] A. Filipponi and A. Di Cicco, “ GNXAS: a software package for advanced EXAFS multiple-scattering calculations and data-analysis”, TASK Quarterly 4, 575-669 (2000), (Poland).
- 3] Nodoka Hara, Andrea Di Cicco, Georghii Tchoudinov, Keisuke Hatada, Calogero Renzo Natoli Relativistic Corrections to Phase Shift Calculation in the GNXAS Package, Symmetry 13, 1021 (2021).
- 4] Georghii Tchoudinov, Andrea Di Cicco, and Calogero Renzo Natoli, Systematic investigation of relativistic effects in EXAFS data analysis, Physical Review B 105, 144109 (2022).