

SPDUST.2

User's guide

Author : Yacine Ali-Haïmoud

March 2010

SPDUST is an IDL program that evaluates the spinning dust emissivity for given, user-provided environmental conditions.

It implements the theoretical formalism presented in the two companion papers:

- Ali-Haïmoud Y., Hirata C. M. & Dickinson C., 2009, MNRAS, 395, 1055 (AHD09),
- Silsbee K., Ali-Haïmoud Y. & Hirata C. M., 2011, MNRAS, 411, 2750 (SAH11).

Please cite the companion papers when using the code as part of any published work.

This version (second release) calculates the emitted spectrum when the smallest, disc-like, grains are not rotating around their axis of greatest inertia (SAH11). It can also calculate the spectrum when the disk-like grains are rotating around their axis of greatest inertia (as in the first release, AHD09).

Please send your questions or comments to yacine@tapir.caltech.edu.

Contents

1	Contents of the package	2
1.1	Contents of <code>SpDust_IDL_routines</code>	2
1.2	Contents of <code>Data_Files</code>	3
2	Basic use of SPDUST	3
2.1	Before running the code	3
2.2	Syntax and examples	4
2.3	Options	5
2.4	How to use an input file	5
2.5	How to run SPDUST on a grid of parameters	6
3	Advanced use	6
3.1	Evaporation temperature T_{ev}	6
3.2	Ambiant radiation field u_ν	6
3.3	Grain optical properties	7
3.4	Inplane to total dipole moment ratio	7
4	Revision history	7

1 Contents of the package

- `Readme.pdf` : this file.
- `SpDust_IDL_routines` : contains the IDL routines of the code.
- `Data_Files` : contains various data files.

1.1 Contents of `SpDust_IDL_routines`

This program uses 10 IDL files, each of which is commented for an easier use.

- `compile_spdust.pro`
IDL batch script to compile all IDL programs. It also reads various files and stores the arrays they contain for later use (in order to speed up the program, some functions were tabulated).
IMPORTANT : you need to change the path for the folder `Data_Files` in this file. For example, if you have downloaded the code in your home directory, you should have after the common blocks :
`SpDust_data_dir = '~/SPDUST.2/Data_Files/'`
- `subroutines.pro`
Contains a few array-creation and interpolation routines used throughout the program.
- `grain_properties.pro`
Contains dust grain physical and geometrical properties (shape, size distribution, dipole moments), along with cgs constants (section 3 of AHD09).
- `charge_dist.pro`
Gets the photoelectric emission rate (Weingartner & Draine 2001a), electron and ion collisional charging rates (Draine & Sutin 1987), to calculate the dust grain charge distribution function.
- `collisions.pro`
Calculates the rotational excitation and damping rates through collisions with neutral species and ions (sections 5 of AHD09 and 7 of SAH11).
- `plasmadrag.pro`
Calculates the rotational excitation and damping rates through interaction with passing ions (sections 6 of AHD09 and 5 of SAH11).
- `infrared.pro`
Calculates the rotational excitation and damping rates through infrared emission (section 7 of AHD09 and 6 of SAH11). The infrared spectrum is obtained following Draine & Li (2001).
- `H2_photoemission.pro`
Calculates the rotational excitation and damping rates through H₂ formation and photoelectric emission (sections 8 and 9 of AHD09).
- `emissivity.pro`
Uses the previously calculated rotational excitation and damping rates to get the rotational distribution function, solution of the Fokker-Planck equation (sections 2 and 4 of AHD09, 3 and 4 of SAH11).

- `SpDust.pro`

Main program. Allows the user to enter the environmental conditions in the form of a structure, and prints out the resulting spectrum in an output file.

NOTE : the program also makes use of the routine `readcol.pro` from the IDL astronomy library (<http://idlastro.gsfc.nasa.gov/>).

This folder also contains two example files :

- `input_file` : example input parameters.
- `nh_grid.pro` : example IDL routine to run `SPDUST` on a grid of number densities.

1.2 Contents of Data_Files

- `PAHneu_read.out`, `PAHion_read.out` : PAH-graphite cross sections for ionized grains, taken from Bruce T. Draine's webpage (<http://www.astro.princeton.edu/~draine/> and references therein).
- `parallel.out`, `perpendicular.out` : parallel and perpendicular refractive indices, taken from Bruce T. Draine's webpage.
- `sizedists_table1.out` : table 1 of Weingartner & Draine (2001b). Contains the parameters for the grain size distribution.
- `FIR_integral_charged_30a_30chi`, `FIR_integral_neutral_30a_30chi`, `GIR_integral_charged_30a_30chi`, `GIR_integral_neutral_30a_30chi` : tables of integrals used in `infrared.pro`.
- `gp_neg_110psi_1500mega`, `gp_pos_110psi_1500mega`, `gp_neutral_300phi_1500mega` : tables of integrals used in `plasmadrag.pro`.
- `Tev_30a_30chi` : table of evaporation temperatures, used in `collisions.pro`. See Section 5.1.4 of AHD09.
- `gff.dat` : table of free-free Gaunt factors taken from Ralf S. Sutherland's webpage (<http://www.mso.anu.edu.au/~ralph/> and references therein).

2 Basic use of SPDUST

2.1 Before running the code

The first thing you need to do is to change the path for the folder `Data_Files` in the file `compile_spdust.pro`. For example, if you have downloaded the code in your home directory, you should edit the file `compile_spdust.pro`, and replace the line (just after the common blocks)

```
SpDust_data_dir = 'path/SPDUST.2/Data_files'
```

by

```
SpDust_data_dir = '~/SPDUST.2/Data_files'
```

You can now open an IDL session from the `SPDUST.2/SpDust_IDL_routines` directory and compile all the routines (and read precalculated tables) by typing :

```
IDL> @compile_spdust
```

This just takes a few seconds on a ~ 2 GHz processor. You just need to do it once for every session.

2.2 Syntax and examples

The main routine of the program is `SPDUST`. The basic syntax to calculate the spinning dust emissivity for given input parameters is as follows :

```
SPDUST, input_parameters, 'path/output_file' [, /case1] [, options]
```

The argument `input_parameters` contains the user-provided environmental and grain parameters, in the form of a structure (see example below), and the argument `'path/output_file'` is the full path of the desired output file for the resulting spinning dust emissivity. The default is to assume that the disklike grains are randomly oriented with respect to their angular momentum axis (as described in SAH11). The optional keyword `/case1` makes the calculation run under the assumption that the grains are spinning around their axis of greatest inertia (just like in the first version of the code).

You need to provide the following input parameters :

- total hydrogen number density n_{H} (in cm^{-3})
- gas temperature T (in K)
- intensity of the radiation field relative to the average interstellar radiation field χ
- hydrogen ionization fraction $x_{\text{H}} \equiv n_{\text{H}^+}/n_{\text{H}}$
- ionized carbon fractional abundance $x_{\text{C}} \equiv n_{\text{C}^+}/n_{\text{H}}$
- molecular hydrogen fractional abundance $y \equiv 2n(\text{H}_2)/n_{\text{H}}$
- H_2 formation efficiency γ (optional, the default is no H_2 formation)
- rms dipole moment for dust grains : either $\mu(a = 10^{-7})$ cm (tag `dipole`) or β , average dipole moment per atom, tag `beta` (both in debye)
- parameters for the grain size distribution : provide the corresponding line of table 1 of Weingartner & Draine (2001b) (starting at one) under the tag `line`

It is preferable to enter all parameters as doubles (suffix `d`), except for `line`, which is an integer.

Example :

```
IDL> input_params = {nh: 30d, T: 1d2, chi: 1d, xh: 1d-3, xc: 3d-4, y: 0d, gamma: 0d,
dipole: 9.3d, line: 7}
```

Or, if you prefer using β , average dipole moment per atom, instead of $\mu(a = 10^{-7})$ cm :

```
IDL> input_params = {nh: 30d, T: 1d2, chi: 1d, xh: 1d-3, xc: 3d-4, y: 0d, gamma: 0d,
beta: 0.38d, line: 7}
```

The tags can be entered in any order and are case-insensitive but all of them must be present, except for the optional `gamma`. Make sure you use the symbol `:` between the tag names and the tag values. Now you can compute the spinning dust emissivity per H atom with the command

```
IDL> SPDUST, input_params, '~/emiss.out'
```

The resulting emissivity per H atom will be printed to the output file you provided (in the example, `~/emiss.out`).

Such a calculation usually takes 10 to 15 seconds on a ~ 2 GHz processor.

2.3 Options

- *Frequency range.*

The default output is given for 200 frequencies logarithmically spaced between 0.5 (used to be 0.01 in SPDUST.1) and 500 GHz. You can change the frequency range and number with the optional keywords `min_freq`, `max_freq` and `N_freq`. For example :

```
IDL> SPDUST, input_params, '~/emiss.out', min_freq = 1d, max_freq = 300d, N_freq = 500
```

Note that `min_freq` and `max_freq` have to be specified in GHz.

- *Free-free emissivity.*

The code can also return the free-free emissivity per H atom corresponding to the given environmental conditions, for an easier comparison (the free-free gaunt factor is taken from Sutherland (1998)). You may set that by using the keyword `/freefree`. For example :

```
IDL> SPDUST, input_params, '~/emiss.out', /freefree
```

- *Number of dipole moments used.*

The spectrum is obtained by averaging over a gaussian distribution of dipole moments with the rms value specified by the user. The default setup is to sum over 20 values of the dipole moment (usually largely sufficient). If the spectrum looks bumpy, you may want to increase to number of values averaged over. This can be done by the keyword `Ndipole`. For example, the command

```
IDL> SPDUST, input_params, '~/emiss.out', Ndipole = 30
```

makes the program average over 30 values of the dipole moment.

- *Verbose mode.*

If you want to get some basic information about grain charge, and rotational excitation and damping mechanisms, and possibly important uncertainty, you can use the keyword `/verbose`.

2.4 How to use an input file

If you prefer having the input parameters in an input file, you can proceed as follows. Modify the example input file provided with the code (`input_file`) to include the environmental parameters you wish to use. For example :

```
input_params = {nh: 30d, T: 1d2, chi: 1d, xh: 1d-3, xc: 3d-4, y: 0d, gamma: 0d,
dipole: 9.3d, line: 7}
```

Once you have saved the new file, you can type at the command line

```
IDL> @input_file
```

This is equivalent to typing the content of the input file at the command line. The structure containing your input parameters, `input_params`, is now defined and you can run as before

```
IDL> SPDUST, input_params, '~/emiss.out'
```

2.5 How to run SPDUST on a grid of parameters

The structure form for the input parameters makes it easy to change one or several parameters without re-defining everything. Each tag can be accessed by `input_paramaters.tag`. For example, if you wish to study the effect of increasing the temperature, all other parameters being unchanged, you can type :

```
IDL> input_params.T = 200d
IDL> SPDUST, input_params, '~/emiss_T200.out'
```

An example file `nh_grid.pro` is provided to show how to run SPDUST on a grid of number densities.

3 Advanced use

3.1 Evaporation temperature T_{ev}

The model for the evaporation temperature used in the code is described in section 5.1.4 of the paper. T_{ev} is calculated for a given grain radius and intensity of the radiation field. The model is physically motivated but its validity is not established. The user may want to use instead a constant evaporation temperature. This can be done by including it as an extra parameter under the tag `Tev` in the input parameters.

Example :

```
IDL> input_params = {nh: 30d, T: 1d2, chi: 1d, xh: 1d-3, xc: 3d-4, y: 0d,
dipole: 9.3d, line: 7, Tev: 20d}
IDL> SPDUST, input_params, '~/emiss.out'
```

3.2 Ambient radiation field u_ν

The radiation field is assumed to be a multiple χ of the average interstellar radiation field defined by Mezger, Mathis & Panagia (1982) and Mathis, Mezger & Panagia (1983). The radiation field comes into the calculation of the grain charge distribution function, through the photoelectric ejection rate, and the excitation and damping rates through infrared emission and photoelectric emission.

The user may want to use a different spectrum. This is possible but the code is not optimized for that. The user willing to do so will need the following information :

- The average interstellar radiation field is defined in the file `charge_dist.pro`, under the function `nu_uisrf` (this returns $\nu \times u_\nu$).
- The photoejection rate $J_{pe}(a, Z)$ is tabulated by the routine `JPEisrf_calc`. If you change `nu_uisrf`, make sure you run `JPEisrf_calc` afterward.
- The infrared emission damping and excitation rates, F_{IR} and G_{IR} , depend upon integrals involving the infrared emission spectrum of the grain. Getting the infrared spectrum requires the calculation of

the probability distribution for the energy levels of the grain, which is a long numerical calculation. This has been done and stored for the average interstellar radiation field. The user can re-do these calculations by running `compute_FGIR_integrals` after changing the spectrum for the radiation field. Depending on the grid of grain radii and radiation intensities used (set up this in `set_up_IR_arrays`), this may take a few days of calculation on a ~ 2 GHz processor.

3.3 Grain optical properties

The absorption efficiencies $Q_{\text{abs}}(a, \nu)$ for the PAH-graphite model are taken from Bruce T. Draine webpage. They are read by the routine `readPAH` in the file `charge_dist.pro`. They are used for the charge distribution function and for the excitation and damping rate due to infrared emission. They can be changed in principle, although, as in the case of the radiation field, this will require re-calculating tables of integrals (see previous section).

3.4 Inplane to total dipole moment ratio

The default is to assume that $\langle \mu_{\text{ip}}^2 \rangle / \langle \mu^2 \rangle = 2/3$. However, if you feel strongly that the dipole moments of PAHs should be oriented differently, you can change this ratio through the tag `inplane` in the input parameters.

For example,

```
IDL> input_params = {nh: 30d, T: 1d2, chi: 1d, xh: 1d-3, xc: 3d-4, y: 0d,
dipole: 9.3d, line: 7, inplane = 0.5d}
IDL> SPDUST, input_params, '~/emiss.out'
```

will compute the spectrum assuming that $\langle \mu_{\text{ip}}^2 \rangle / \langle \mu^2 \rangle = 1/2$ for the disklike grains.

4 Revision history

December 2008 : first release.

March 2010 : second release, implementing rotation of disklike grains around a non-principal axis. Other minor changes are documented in the routines themselves.

References

- The seminal papers that first suggested spinning dust as a possible origin for anomalous emission are:
Draine B., Lazarian A., 1998a, ApJ, 494, L19
Draine B., Lazarian A., 1998b, ApJ, 508, 157
- Papers cited in this readme file (see AHD09 and SAH11 for more references):
Draine B. T. & Li A., 2001, ApJ, 554, 778
Draine B. T. & Sutin B., 1987, ApJ, 320, 803
Mathis J., Mezger P. & Panagia M., 1983, A&A, 128, 212
Mezger P., Mathis J. & Panagia M., 1982, A&A, 105, 372
Sutherland R., 1998, MNRAS, 300, 321
Weingartner J. & Draine B. T., 2001a, ApJS 134, 263
Weingartner J. & Draine B. T., 2001b, ApJ, 548, 296