The hac.out output file

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Brief Description

This file contains the heat current auto-correlation (HAC) function and the running thermal conductivity (RTC) from the EMD (Green-Kubo) method.

The keyword which produces the current file

- compute_hac in run.in

File format

- This file reads:
  - column 1: correlation time (in units of ps)
  - column 2: $\left\langle J_x^{\rm in}(0) J_x^{\rm tot}(t) \right\rangle$ (in units of eV^3/amu)
  - column 3: $\left\langle J_x^{\rm out}(0) J_x^{\rm tot}(t) \right\rangle$ (in units of eV^3/amu)
  - column 4: $\left\langle J_y^{\rm in}(0) J_y^{\rm tot}(t) \right\rangle$ (in units of eV^3/amu)
  - column 5: $\left\langle J_y^{\rm out}(0) J_y^{\rm tot}(t) \right\rangle$ (in units of eV^3/amu)
  - column 6: $\left\langle J_z^{\rm tot}(0) J_z^{\rm tot}(t) \right\rangle$ (in units of eV^3/amu)
  - column 7: $\kappa_x^{\rm in}(t)$ (in units of W/mK)
  - column 8: $\kappa_x^{\rm out}(t)$ (in units of W/mK)
  - column 9: $\kappa_y^{\rm in}(t)$ (in units of W/mK)
  - column 10: $\kappa_y^{\rm out}(t)$ (in units of W/mK)
  - column 11: $\kappa_z^{\rm tot}(t)$ (in units of W/mK)
- Note that the HAC and the RTC have been decomposed as described in this paper (https://doi.org/10.1103/PhysRevB.95.144309). This decomposition is useful for 2D materials but is not necessary for 3D materials. For 3D materials, one can sum up some columns to get the conventional data. For example:

$$\left\langle J_x^{\rm tot}(0) J_x^{\rm tot}(t) \right\rangle = \left\langle J_x^{\rm in}(0) J_x^{\rm tot}(t) \right\rangle + \left\langle J_x^{\rm out}(0) J_x^{\rm tot}(t) \right\rangle.$$

$$\kappa_x^{\rm tot}(t) = \kappa_x^{\rm in}(t) + \kappa_x^{\rm out}(t).$$

- Note that the *cross term* introduced in the above paper (https://doi.org/10.1103/PhysRevB.95.144309) has been evenly attributed to the in- and out-of-plane components. This has been justified in this paper (h

ttps://doi.org/10.1103/PhysRevB.99.064308).

Tips

- Only the potential part of the heat current has been included. If the convective part of the heat current is important in your system, you can use the compute keyword to calculate and output the heat current data and post-process by yourself.
