The compute shc keyword

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Purpose

- The `compute_shc` keyword is used to compute the non-equilibrium virial-velocity correlation function $K(t)$ and the spectral heat current (SHC) $J_q(\omega)$, in a given direcction, for a group of atoms, as defined in Eq. (18) and the left part of Eq. (20) of [Fan 2019].

Grammar

```
compute_shc sample_interval Nc transport_direction num_omega max_omega <options>
```

- `sample_interval` is the sampling interval (number of steps) between two correlation steps. This parameter must be an integer that is ≥ 1 and ≤ 10.
- `Nc` is the total number of correlation steps. This parameter must be an integer that is ≥ 100 and ≤ 1000.
- `transport_direction` is the direction of heat transport to be measured. It can only be 0, 1, and 2, corresponding to the x, y, and z directions, respectively.
- `num_omega` is the number of frequency points one wants to consider.
- `max_omega` is the maximum **angular frequency** (in units of THz) one wants to consider. The angular frequency data will be `max_omega/num_omega, 2*max_omega/num_omega, ..., max_omega`.
- `<options>` can only be `group`, which requires two parameters:

```
group grouping_method group_id
```

This meas that $K(t)$ will be calculated for atoms in group `group_id` of grouping method `grouping_method`. Here `group_id` should ≥ 0 and smaller than the number of groups in grouping method `grouping_method`. Also, grouping method `grouping_method` must be defined in the xyz.in file. If this option is missing, it means computing $K(t)$ for the whole system.

Examples

Example 1

- The command

```
compute_shc 2 250 0 1000 400.0
```

means that

- you want to calculate $K(t)$ for the whole system;
- the sampling interval is 2;
- the maximum number of correlation steps is 250;
- the transport direction is x;
- you want to consider 1000 frequency points;
- the maximum angular frequency is 400 THz.

Example 2

- The command

```
compute_shc 1 500 1 500 200.0 group 0 4
```

means that

- you want to calculate $K(t)$ for atoms in group `4` defined in grouping method `0`;
- the sampling interval is 1 (sample the data at each time step);
- the maximum number of correlation steps is 500;
- the transport direction is y;
- you want to consider 500 frequency points;
- the maximum angular frequency is 200 THz.

Caveats

- This computation can be memory consuming.

Output file

- shc.out

Related tutorial

- Tutorial: Thermal transport from NEMD and HNEMD

References

- [Fan 2019] Zheyong Fan, Haikuan Dong, Ari Harju, and Tapio Ala-Nissila, *Homogeneous nonequilibrium molecular dynamics method for heat transport and spectral decomposition with many-body potentials* (https://doi.org/10.1103/PhysRevB.99.064308), Phys. Rev. B **99**, 064308 (2019).

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