The shc.out output file

From GPUMD
Jump to navigationJump to search

Contents

- 1 Brief description
- 2 The keyword which produces the current file
- 3 File format
- 4 Tips
- 5 References

Brief description

- This file contains 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].

The keyword which produces the current file

- compute_shc

File format

- For each run, there are 3 columns and `2*Nc-1 + num_omega` rows. Here, `Nc` is the number of correlation steps and `num_omega` is the number of frequency points.
- In the first `2*Nc-1` rows:
  - column 1: correlation time t, from negative to positive, in units of ps;
  - column 2: $K^{\rm in}(t)$ in units of A*eV/ps;
  - column 3: $K^{\rm out}(t)$ in units of A*eV/ps.
- $K^{\rm in}(t) + K^{\rm out}(t) = K(t)$ is exactly the expression in Eq. (18) of [Fan 2019]. The in-out decomposition follows the definition in [Fan 2017], which is useful for 2D materials but is not necessary for 3D materials.
- In the next `num_omega` rows:
  - column 1: angular frequency ω, in units of THz;
  - column 2: $J_q^{\rm in}(\omega)$ in units of A*eV/ps/THz;
  - column 3: $J_q^{\rm out}(\omega)$ in units of A*eV/ps/THz.
- $J_q^{\rm in}(\omega) + J_q^{\rm out}(\omega) = J_q(\omega)$ is exactly the left expression in Eq. (20) of [Fan 2019].

Tips

- Only the potential part of the heat current has been included.

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).
- [Fan 2017] Zheyong Fan, Luiz Felipe C. Pereira, Petri Hirvonen, Mikko M. Ervasti, Ken R. Elder, Davide Donadio, Tapio Ala-Nissila, and Ari Harju, *Thermal conductivity decomposition in two-dimensional materials: Application to graphene* (https://doi.org/10.1103/PhysRevB.95.144309), Phys. Rev. B **95**, 144309 (2017).