SPARC - SQ

Spectral Quadrature method

User guide

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Contributors
Citation
Acknowledgements

Contributors

- **Phanish Suryanarayana** (PI)
  - **Xin Jing**: Code infrastructure
  - **Abhiraj Sharma**: Initial development
  - **Phanisri P. Pratapa**: Initial development
- **John E. Pask** (co-PI)

Citation

If you publish work using/regarding SPARC-SQ, please cite the following articles, in addition to SPARC citations:

- https://doi.org/10.1016/j.cpc.2015.11.005 (initial implementation),
  https://doi.org/10.1016/j.cplett.2013.08.035 (formulation),
  https://doi.org/10.1007/978-3-031-22340-2_12 (detailed mathematical formulation),

Acknowledgements

- **U.S. Department of Energy (DOE), National Nuclear Security Administration (NNSA): DE-NA0004128**

Comments

The code will fail with the following options and the related input options are listed.

- Polarized calculation: `SPIN_TYP`.
- K-point calculation: `KPOINT_GRID`, `KPOINT_SHIFT`.
- Dirichlet boundary condition in any direction: `BC`
- Define number of states/orbitals: `NSTATES`
- Print eigenvalues into file: `PRINT_EIGEN`

Input file options

Spectral Quadrature

SQ_AMBIENT_FLAG | SQ_HIGHT_FLAG | SQ_RCUT | SQ_NPL_G | SQ_HIGHT_GAUSS_HYBRID_MEM | SQ_TOL_OCC | NP_DOMAIN_SQ_PARAL

Spectral Quadrature

SQ_AMBIENT_FLAG

Type

Integer

Unit

No unit

Default

0

Example

```
SQ_AMBIENT_FLAG: 1
```

Description

Flag to turn on SQ method

Remark

SQ method can not be turned on simultaneously with CS, SQ3, hybrid functionals.

SQ_HIGHT_FLAG

Type

Integer

Unit

No unit

Default

0

Example

```
SQ_HIGHT_FLAG: 1
```

Description

Flag to turn on SQ method for High Temperature

Remark

At High Temperature, spin-polarized calculation is not supported and high memory usage is always enabled. To use Low Temperature SQ method, please turn it off by setting SQ_HIGHT_FLAG: 0.

SQ_RCUT

Type

Double

Unit

Bohr

Default

None

Example

`SQ_RCUT: 2.0`

Description

Truncation or localization radius

Remark

`SQ_RCUT` must be specified if SQ is turned on.

SQ_NPL_G

Type

Integer

Unit

No unit

Default

None

Example

SQ_NPL_G: 24

Description

Degree of polynomial for Gauss Quadrature.

Remark

SQ_NPL_G must be specified if SQ is turned on.

SQ_HIGHT_GAUSS_HYBRID_MEM

Type

String

Unit

No unit

Default

LOW

Example

SQ_HIGHT_GAUSS_HYBRID_MEM: HIGH

Description

Flag for memory option when using Gauss quadrature at High Temperature for saving the exact exchange potential when using hybrid functionals.

SQ_TOL_OCC

Type

Double

Unit

No unit

Default

10^{-6}

Example

SQ_TOL_OCC: 1E-5

Description

Tolerance for occupation corresponding to maximum eigenvalue.

NP_DOMAIN_SQ_PARAL

Type

Integer

Unit

No unit

Default

Automatically optimized

Example

`NP_DOMAIN_SQ_PARAL`: 3 3 2

Description

Dimensions of the 3D Cartesian topology for SQ method.

Remark

This option is for development purpose. It's better to let SPARC choose the parallization parameters in practice.