RSDFT User Guide

Ver. 1.0

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1 Basics of Solid-state Physics

This chapter describes the basics necessary to calculate the electronic structure and defines related terms and symbols.

1.1 Atomic Units

In accordance with conventional practices, Hartree atomic units $(\hbar = m_e = e^2 = 1)$ are used to calculate the electronic structure, except for the cut-off energy, which is calculated in Rydberg atomic units.

Length	1 bohr = 0.5291772083 Å
Energy	1 hartree = 27.21138344 eV
	1 Ry = 0.5 hartree = 13.60569172 eV
Time	1 a.u. = 0.0241888433 fs

In addition, the following are often used for unit conversions and other relevant calculations:

Boltzmann constant 1 k_B = 0.08617342 meV/K

Energy 1 kcal/mol = 0.04337 eV

1.2 Unit Cells

1.2.1 Real Lattice Vectors

A real lattice vector is given by specifying the three vector components, which form the edges of the unit cell in a crystal: x, y, and, z.

$$\mathbf{a}_1 = \begin{pmatrix} a_1^x \\ a_1^y \\ a_1^z \end{pmatrix} \qquad \mathbf{a}_2 = \begin{pmatrix} a_2^x \\ a_2^y \\ a_2^z \end{pmatrix} \qquad \mathbf{a}_3 = \begin{pmatrix} a_3^x \\ a_3^y \\ a_3^z \end{pmatrix} \tag{1.1}$$

Any translation vector in real space can be expressed using integers m_1, m_2, m_3 as

$$\mathbf{R} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3 \tag{1.2}$$

1.2.2 Reciprocal Lattice Vectors and the Brillouin Zone

The following are reciprocal lattice vectors

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \tag{1.3}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \tag{1.4}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \tag{1.5}$$

The volume of a Brillouin zone (BZ) is given by

$$\Omega_{BZ} = \mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{(2\pi)^3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = \frac{(2\pi)^3}{\Omega_{cell}} \tag{1.6}$$

The volume element in the BZ, which is also called the k-space, is expressed as

$$\Delta\mathbf{k} = \frac{\Omega_{BZ}}{N_{cell}} = \frac{(2\pi)^3}{N_{cell}\Omega_{cell}} = \frac{(2\pi)^3}{\Omega_{crystal}} \tag{1.7}$$

Any translation vector in reciprocal space can be expressed using integers n_1, n_2, n_3 as

$$\mathbf{G} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3 \tag{1.8}$$

Additionally, any point in the BZ can be expressed using real numbers k_1, k_2, k_3 as

$$\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3 \tag{1.9}$$

where vector $\mathbf{k}$ is the wave number of the Bloch function, which is given by

$$\phi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{1.10}$$

Vector $\mathbf{k}$ indicates the direction and wave number (the reciprocal of the wavelength) of the waveform for a wave propagating across multiple unit cells in a crystal. Vector $\mathbf{G}$ is the wave number for the base function in the plane wave expansion, and is given by

$$u_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} c_{n\mathbf{k}}(\mathbf{G})e^{i\mathbf{G}\cdot\mathbf{r}} \tag{1.11}$$

Equation (1.11) represents detailed changes in the waveform (with a short wavelength) within the range of the unit cell. The maximum size of $\mathbf{G}$, which is used as the base function, is called the cut-off wave number, or cut-off for short, and its square is called the cut-off energy. In calculations using the plane wave expansion method, the plane wave with a wave number in the range given below is used as the base function.

$$\begin{gathered} |\mathbf{G}| \le G_{cut} \\ |\mathbf{G}|^2 \le E_{cut} \quad \text{(Ry)} \end{gathered} \tag{1.12}$$

1.2.3 Real-space Grid

As is well known in Fourier analysis, determining the cut-off wave number also regulates the resolution of the corresponding real-space grid in order to prevent errors due to “aliasing”. Conversely, in the real-space method, the resolution (i.e., the number of grid points to discretize the space in a unit cell) is specified in advance. The number of grid points is determined by the number of sections that each side of the unit cell is divided. Increasing the number of divisions (i.e., reducing the grid spacing) improves the calculation accuracy. This is equivalent to increasing the cut-off energy in plane wave calculations. The cut-off and real-space grid spacing Δ have the following relationship

$$G_{cut} \approx \frac{\pi}{\Delta} \tag{1.13}$$

Equation (1.13) is similar to the Nyquist frequency, which is the maximum frequency that a signal with a finite time increment can be transmitted. Because RSDFT uses the same grid for wave functions and density/potential, it is essential to secure a grid width so that it can handle slightly larger cut-offs than those considered to be sufficient in the plane wave calculations while being mindful of the convergence of the calculation results with respect to grid width.

1.2.4 Atomic Coordinates

The atomic coordinates in a unit cell are often represented directly as the x, y, and z components (xyz-representation) or in the basis of the real lattice vectors (a-representation or lattice-coordinate representation).

$$\begin{aligned}\mathbf{R}_{\mathrm{ion}} &= X_{\mathrm{ion}}\mathbf{e}_x + Y_{\mathrm{ion}}\mathbf{e}_y + Z_{\mathrm{ion}}\mathbf{e}_z \\ &= \alpha^1_{\mathrm{ion}}\mathbf{a}_1 + \alpha^2_{\mathrm{ion}}\mathbf{a}_2 + \alpha^3_{\mathrm{ion}}\mathbf{a}_3\end{aligned} \tag{1.14}$$

The coordinate components in these two representation methods have the following relationship

$$\begin{pmatrix} X_{\mathrm{ion}} \\ Y_{\mathrm{ion}} \\ Z_{\mathrm{ion}} \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3 \end{pmatrix} \begin{pmatrix} \alpha^1_{\mathrm{ion}} \\ \alpha^2_{\mathrm{ion}} \\ \alpha^3_{\mathrm{ion}} \end{pmatrix} \tag{1.15}$$

1.3 Brillouin Zone Integration (K-point Sampling)

In various situations of solid-state physics, the following integral must be evaluated

$$I = \int_{\Omega_{BZ}} f(\mathbf{k})\,d\mathbf{k} \tag{1.16}$$

Numerically, equation (1.16) can be approximated by the sum of a finite number of k-points in the BZ.

$$I \approx \sum_{\mathbf{k}}^{\mathrm{BZ}} w(\mathbf{k}) f(\mathbf{k}) \Delta\mathbf{k} \tag{1.17}$$

Therefore, it is essential to obtain a better integral approximation using the fewest possible number of k-points. The special-points method is an approach to improve the approximation accuracy via the selection of the k-points.

Normally $f(\mathbf{k})$ is used to deal with periodic functions in reciprocal space as

$$f(\mathbf{k}+\mathbf{G}) = f(\mathbf{k}) \tag{1.18}$$

However, periodic functions can also be expressed using a Fourier series expression as

$$f(\mathbf{k}) = \sum_{\mathbf{R}} f(\mathbf{R}) e^{i\mathbf{k}\cdot\mathbf{R}} \tag{1.19}$$

Using equation (1.19), the BZ integration (1.16) becomes

$$I = \sum_{\mathbf{R}} f(\mathbf{R}) \int_{\Omega_{BZ}} e^{i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k} = \Omega_{BZ} f(\mathbf{R}=0) \tag{1.20}$$

Consider a calculation using the discrete sum (equation (1.17)). If a set of k-points that satisfies equation (1.21) for all real lattice vectors with $\mathbf{R} \neq 0$ exists, then the rigorous integration results can be reproduced using equation (1.17).

$$\sum_{\mathbf{k}}^{BZ} w(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{R}} = 0 \tag{1.21}$$

However, achieving this with a finite number of such k-points is impossible. As a realistic alternative, an approximation with a set of a finite number of k-points that satisfies equation (1.21) "for as many real lattice vectors as possible" is used. Currently, any term on the right side of equation (1.19) that includes one or more real lattice vectors that do not satisfy equation (1.21) results in an error.

In the case of a metallic system, in addition to an integration that includes the entire BZ as in equation (1.16), equation (1.23) must be calculated such that the integration integral is inside the curved surface (Fermi surface), which is defined by equation (1.22).

$$\varepsilon(\mathbf{k}) = \varepsilon_F \tag{1.22}$$

$$I = \int_{\varepsilon(\mathbf{k}) \le \varepsilon_F} f(\mathbf{k})\, d\mathbf{k} \tag{1.23}$$

For this type of numerical calculation of an integral, the smearing or tetrahedron method is used.

1.4 Density Functional Theory

This section provides a brief description of density functional theory (DFT), which is the basic theory of calculus.

1.4.1 Kohn–Sham Equations

Consider the following equation without spin freedom

$$\left(-\frac{1}{2}\nabla^2 + v_{loc}(\mathbf{r}) + \hat{v}_{nloc}^{pp} \right) \phi_n(\mathbf{r}) = \varepsilon_n \phi_n(\mathbf{r}) \tag{1.24}$$

where the local potential is the sum of the Hartree potential, the XC potential, and the local pseudopotential. The Hartree potential and the XC potential depend on the electron density (or the Kohn–Sham orbitals).

$$v_{loc}(\mathbf{r}) = v_{hartree}(\mathbf{r}) + v_{xc}(\mathbf{r}) + v_{loc}^{pp}(\mathbf{r}) \tag{1.25}$$

A non-local potential derived from only the pseudopotential can be defined generally as the operator, which is given as

$$\hat{v}_{nloc}^{pp}\phi_n(\mathbf{r}) = \int d\mathbf{r}' v_{nloc}^{pp}(\mathbf{r},\mathbf{r}')\phi_n(\mathbf{r}') \tag{1.26}$$

If a separable approximation of the norm-conserving pseudopotential is used, then the operator is expressed as

$$\hat{v}_{nloc}^{pp}\phi_n(\mathbf{r}) = \sum_{a=1}^{N_{atom}} \sum_{l=0}^{l_{\max}} \sum_{m=-l}^{l} c_{alm}\beta_{alm}^{pp}(\mathbf{r}) \int d\mathbf{r}' \beta_{alm}^{pp}(\mathbf{r}')\phi_n(\mathbf{r}') \tag{1.27}$$

However, equation (1.27) can be formally expressed in the form shown in equation (1.26). In the case of solids (periodic systems), although an equation to obtain a Bloch function (1.10) can also be considered

$$\left(-\frac{1}{2}\nabla^2 + v_{loc}(\mathbf{r}) + \hat{v}_{nloc}^{pp}\right)\phi_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_{n\mathbf{k}}\phi_{n\mathbf{k}}(\mathbf{r}) \tag{1.28}$$

RSDFT is designed to solve the following equation for the periodic function portion $u_{n\mathbf{k}}$

$$\left(-\frac{1}{2}\nabla^2 - i\mathbf{k}\cdot\nabla + \frac{k^2}{2} + v_{loc}(\mathbf{r}) + e^{-i\mathbf{k}\cdot\mathbf{r}}\hat{v}_{nloc}^{pp}e^{i\mathbf{k}\cdot\mathbf{r}}\right)u_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_{n\mathbf{k}}u_{n\mathbf{k}}(\mathbf{r}) \tag{1.29}$$

(Note that differentiating these two equations makes them non-equivalent.) Normalization can be performed as

$$\int_{\Omega_{cell}} d\mathbf{r}\left|\phi_{n\mathbf{k}}(\mathbf{r})\right|^2 = \int_{\Omega_{cell}} d\mathbf{r}\left|u_{n\mathbf{k}}(\mathbf{r})\right|^2 = \left\langle u_{n\mathbf{k}} \middle| u_{n\mathbf{k}}\right\rangle = 1 \tag{1.30}$$

Although the equations given hereafter are intended for solids, they are exactly the same as for molecules when considering the case where $\mathbf{k} = 0$ (Γ-point). Thus, both cases can be discussed almost in parallel.

The density of electrons is given by

$$n(\mathbf{r}) = \sum_{n\mathbf{k}} f_{n\mathbf{k}} \left|\phi_{n\mathbf{k}}(\mathbf{r})\right|^2 = \sum_{n\mathbf{k}} f_{n\mathbf{k}} \left|u_{n\mathbf{k}}(\mathbf{r})\right|^2 \tag{1.31}$$

where $f_{n\mathbf{k}}$ is the occupation number, which indicates that the orbitals are occupied by electrons in order beginning with the smallest eigenvalue that satisfies the following

$$\begin{gathered} 0 \le f_{n\mathbf{k}} \le 2 \\ \sum_{n\mathbf{k}} f_{n\mathbf{k}} = N_{electron} \end{gathered} \tag{1.32}$$

Two methods can be used to calculate equation (1.32). The first expresses this number as a step function that takes 0 or 2 based on the boundary of the Fermi energy

$$f_{n\mathbf{k}} = 2\theta(\varepsilon_{n\mathbf{k}} - \varepsilon_F) \tag{1.33}$$

The second is to approximate it by a smoother function

$$f_{n\mathbf{k}} = 2f(\varepsilon_{n\mathbf{k}} - \varepsilon_F) \tag{1.34}$$

The latter is called the smearing method, which employs the Fermi–Dirac distribution functions, error functions, Hermite polynomials, etc.

Since the potential depends on the electron density, equation (1.24) or (1.28) and equations (1.25) and (1.31) must be solved in a self-consistent manner. This is often called an SCF calculation, which denotes a calculation to obtain a self-consistent field (SCF).

1.4.2 Total Energy

The energy of a system in the ground state can be expressed as

$$E_{total} = T + E_{ee} + E_{ei} + E_{ii} \tag{1.35}$$

Here it is assumed that the kinetic energy contributes only to electron systems (the Born-Oppenheimer approximation) and the last term of the equation is the interaction energy between ions (point charges), which is the Ewald sum in a periodic system.

In DFT, the same energy is expressed as

$$E_{total} = T_s + E_{hartree} + E_{xc} + E_{ei} + E_{ii} \tag{1.36}$$

where the terms other than E_{xc} can be expressed explicitly as

$$T_s = \sum_{n\mathbf{k}} f_{n\mathbf{k}} \left\langle \phi_{n\mathbf{k}} \right| -\frac{1}{2}\nabla^2 \left| \phi_{n\mathbf{k}} \right\rangle \tag{1.37}$$

$$E_{hartree} = \frac{1}{2}\int_{\Omega_{cell}} d\mathbf{r} \int d\mathbf{r}' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \tag{1.38}$$

$$E_{ei} = \int_{\Omega_{cell}} d\mathbf{r} v_{loc}^{pp}(\mathbf{r})n(\mathbf{r}) + \sum_{n\mathbf{k}} f_{n\mathbf{k}} \left\langle \phi_{n\mathbf{k}} \right| \hat{v}_{nloc}^{pp} \left| \phi_{n\mathbf{k}} \right\rangle \tag{1.39}$$

The double integral in equation (1.38) has a limited range because $E_{hartree}$ represents the energy per unit cell. In the case of molecules, Ω_{cell} is regarded as the whole calculation domain (i.e., the whole space). The term Exc is the electron density or a complex function of the Kohn–Sham orbitals and, practically, an approximation function type such as LDA or GGA is set before starting a specific calculation.

Consider a calculation of the minimized orbitals under the condition where the normalization is kept constant (equation (1.36)). In this case, the Kohn–Sham equation (1.28) is the variational equation. The potential at this time is

$$
\begin{aligned}
v_{loc}(\mathbf{r}) &= \frac{\delta E_{hartree}}{\delta n(\mathbf{r})} + \frac{\delta E_{xc}}{\delta n(\mathbf{r})} + \frac{\delta E_{ei}}{\delta n(\mathbf{r})} \\
&= \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \frac{\delta E_{xc}}{\delta n(\mathbf{r})} + v_{loc}^{pp}(\mathbf{r}) \\
&= v_{hartree}(\mathbf{r}) + v_{xc}(\mathbf{r}) + v_{loc}^{pp}(\mathbf{r})
\end{aligned}
\tag{1.40}
$$

Minimizing the energy for the orbitals is equivalent to solving the Kohn–Sham equation in a self-consistent manner.

Next consider calculating the total energy in the middle of the SCF iterations. Assuming that the orbitals obtained after advancing the calculation one step under a given potential $v_{hartree}^{in} + v_{xc}^{in}$ are $\phi_{n\mathbf{k}}^{out}$ and the density calculated from the orbitals is n^{out}, the total energy is given as

$$
E_{total} = \sum_{n\mathbf{k}} f_{n\mathbf{k}} \varepsilon_{n\mathbf{k}} - \int_{\Omega} d\mathbf{r} \left\{ v_{hartree}^{in}(\mathbf{r}) + v_{xc}^{in}(\mathbf{r}) \right\} n^{out}(\mathbf{r}) + E_{hartree}[n^{out}] + E_{xc}[n^{out}] \tag{1.41}
$$

where $\varepsilon_{n\mathbf{k}}$ is the expected value, which is expressed as

$$
\varepsilon_{n\mathbf{k}} = \left\langle \phi_{n\mathbf{k}}^{out} \left| -\frac{1}{2}\nabla^2 + v_{hartree}^{in} + v_{xc}^{in} + v_{loc}^{pp} + \hat{v}_{nloc}^{pp} \right| \phi_{n\mathbf{k}}^{out} \right\rangle \tag{1.42}
$$

Of course, all terms in equation (1.36) can be recalculated using $\phi_{n\mathbf{k}}^{out}$. However, $\varepsilon_{n\mathbf{k}}$ is typically obtained during an iterative calculation. This is more time efficient because the inner product calculations can be eliminated for all orbitals in the system.

There is another type of equation for the total energy called the Harris functional, which is expressed as

$$
E_{total}^{Harris} = \sum_{n\mathbf{k}} f_{n\mathbf{k}} \varepsilon_{n\mathbf{k}} - \frac{1}{2} \int_{\Omega} d\mathbf{r} v_{hartree}^{in}(\mathbf{r}) n^{in}(\mathbf{r}) - \int_{\Omega} d\mathbf{r} v_{xc}^{in}(\mathbf{r}) n^{in}(\mathbf{r}) + E_{xc}[n^{in}] \tag{1.43}
$$

This functional was developed with the expectation of realizing a better approximation to the converged solution in a single step, allowing the SCF iteration process to be bypassed. If a converged solution can be obtained, then (1.36), (1.41), and (1.43) all have the same value.

1.4.3 Hellmann–Feynman Force

The arrangement of atoms (ions) determines the pseudopotential, which subsequently determines the Kohn–Sham equation. Thus, the SCF can be calculated to obtain the energy of an electron system in the ground state under a given arrangement of atoms. One of the most important applications of DFT is to test various arrangements of atoms to determine the structure that minimizes the energy. To efficiently perform such an "atomic structure optimization", it is essential to differentiate the atomic coordinates of the energy as

$$\mathbf{F}_I = -\frac{\partial E_{total}}{\partial \mathbf{R}_I} \tag{1.44}$$

Equation (1.44) can be regarded as the force applied to the i-th atom, which can be used to execute molecular dynamics calculations (first principles molecular dynamics). This differentiation is performed using equation (1.36) as well as equations (1.37) – (1.40). Calculating wave functions and density using the SCF converged solution for each structure yields

$$\mathbf{F}_I = -\int_{\Omega_{cell}} d\mathbf{r} \frac{\partial v_{loc}^{pp}(\mathbf{r})}{\partial \mathbf{R}_I} n(\mathbf{r}) - \sum_{n\mathbf{k}} f_{n\mathbf{k}} \langle \phi_{n\mathbf{k}} | \frac{\partial \hat{v}_{nloc}^{pp}}{\partial \mathbf{R}_I} | \phi_{n\mathbf{k}} \rangle \tag{1.45}$$

This calculation can be performed easily because it does not involve the differentiation of the atomic coordinates for wave functions and density (the Hellmann–Feynman theorem).

1.4.4 Background Charge Correction

This should be considered only when calculating the charge state in a periodic system. In a periodic system, all the energy is released unless the charge is neutral in the unit cell. To avoid this total release of energy, there are cases where a spatially uniform background charge is artificially introduced into the calculations as the number of electrons increase or decrease, resulting in the appearance of several additional terms. The interaction energy with electrons is expressed as

$$E_{ei} + E_{e-bg} = \int_{\Omega_{cell}} d\mathbf{r} v_{loc}^{pp}(\mathbf{r}) n(\mathbf{r}) + \int_{\Omega_{cell}} d\mathbf{r} n(\mathbf{r}) \int d\mathbf{r}' \frac{n_{bg}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \tag{1.46}$$

The following additional term appears due to the second term on the right-hand side.

$$\int_{\Omega_{cell}} d\mathbf{r} n(\mathbf{r}) \int d\mathbf{r}' \frac{n_{bg}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} = \frac{N_{electron} N_{bg}}{\Omega_{cell}} \lim_{G \to 0} \frac{4\pi}{G^2} \tag{1.47}$$

On the other hand, the interaction energy with ions is given by

$$\begin{aligned} E_{ii} + E_{i-bg} + E_{bg-bg} &= \frac{1}{2} \int_{\Omega_{cell}} d\mathbf{r} \int d\mathbf{r}' \frac{\{n_{ion}(\mathbf{r}) + n_{bg}(\mathbf{r})\}\{n_{ion}(\mathbf{r}') + n_{bg}(\mathbf{r}')\}}{|\mathbf{r}-\mathbf{r}'|} \\ &= E_{ewald} \\ &+ \int_{\Omega_{cell}} d\mathbf{r} \int d\mathbf{r}' \frac{n_{ion}(\mathbf{r}) n_{bg}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\ &+ \frac{1}{2} \int_{\Omega_{cell}} d\mathbf{r} \int d\mathbf{r}' \frac{n_{bg}(\mathbf{r}) n_{bg}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \end{aligned} \tag{1.48}$$

The following additional terms appear due to the second and third terms on the right-hand side.

$$\int_{\Omega_{cell}} d\mathbf{r} n_{ion}(\mathbf{r}) \int d\mathbf{r}' \frac{n_{bg}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} = \frac{N_{ion} N_{bg}}{\Omega_{cell}} \lim_{G \to 0} \frac{4\pi}{G^2} \tag{1.49}$$

and

$$\frac{1}{2} \int_{\Omega_{cell}} d\mathbf{r} \int d\mathbf{r}' \frac{n_{bg}(\mathbf{r}) n_{bg}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{2} \frac{N_{bg} N_{bg}}{\Omega_{cell}} \lim_{G \to 0} \frac{4\pi}{G^2} \tag{1.50}$$

These divergent terms work to cancel the divergence of the Hartree term and the local potential terms.

In charge state calculations for point defects, there are cases where multipole interactions between supercells cannot be ignored even if the charge is not neutral in the unit cell. There are also a number of arguments associated with the correction of interactions in such cases.

2 List of implemented functions

2.1 Exchange-Correlation Functionals

- Local-Density Approximation (PZ81, PW92)
- Generalized Gradient Approximation (PBE96, PW91)
- Hybrid Functional (HSE, PBE0, HF)
- van der Waals DFT

2.2 Spin

- Spin-dependent calculations (Non-colinear spin is not available yet)

2.3 Pseudopotentials

- Norm-conserving pseudopotential
- Ultrasoft pseudopotential (only for PSV pseudopotential)

2.4 Functions

- Atomic structure optimization (CG method)
- Band structure calculation
- Band unfolding
- Charged-state calculation

2.5 Boundary conditions

- 3D-periodic boundary condition (We call this code "RSSOL")
- 0D-isolated (or molecular) boundary condition (We call this code "RSMOL")

2.6 Parallelization

- Grid, band, k-point, spin parallelization with MPI
- Thread parallelization for grid with OpenMP
- Hybrid parallelization with MPI and OpenMP

3 Compilation and Execution

3.1 How to Edit `make.inc`

Copy the `make.inc.org` in `src/` as `make.inc` and specify the following:

- Compiler
- Compilation options (including preprocessor options such as `-cpp`)
- Link options
- BLAS, LAPACK, ScaLAPACK
- Keywords to be passed to the preprocessor

Edit the following items in `make.inc` to suit your environment:

`FC =` Compiler
`FFLAGS0 =` Compilation options
`LFGALS0 =` Link options
`OMPFLAG =` Option to compile with OpenMP
`LAPACK_L =` Links to BLAS, LAPACK, and ScaLAPACK
`FFTW_L =` Link to FFTW (if use)
`INCLUDE_DIR =` PATH to the include files
`CPP_FLAGS =` Keywords to be passed to the preprocessor

Several samples are already provided. If the suitable sample exists, you can use just by uncommenting the appropriate lines. Preprocessor option such as `-cpp` is always necessary.

The following can be specified for the keywords to be passed to the preprocessor:

`-D_DRSDFT_`	Creates a double-precision-real version execution module
`-D_FFTE_`	Uses parallel fast Fourier transform `FFTE`
`-D_FFTW_`	Uses parallel fast Fourier transform `FFTW`
`-D_LAPACK_`	Uses LAPACK without ScaLAPACK

Currently, only the double-precision-real version supports the execution of molecule-version

(RSMOL) calculations.

3.2 Input Files

The following input files are required to execute the program:

`fort.1`	Description of various parameters required for execution
`fort.2`	Parameters required only to execute molecule-version (RSMOL) calculations
`fort.970`	Initial configuration of atoms
`fort.980`	Required only to specify the initial spin configuration for spin calculations
`Pseudopotential`	File name is described in fort.1
`wf.dat1*`	Only required to read the wave function obtained by the previous calculation
`vrho.dat1`	Only required to read the results of the previous density/potential calculation
`wopt.dat`	Only required to take over the structure optimization history to restart the calculation

Note that fort.1, fort.970, and pseudopotential files are always required.

3.3 Execution

In the directory where the input files (e.g., fort.1) are located, execute a command such as

```
mpirun -np Number of Processes ./a.out
```

3.4 Output Files

Once the calculation is complete, the following files may be generated:

`fort.99`	Final results of the total energy, eigenvalues
`fort.97`	Atomic coordinates during a line-minimization search in structure optimization
`fort.197`	Atomic coordinates after completion of a line-minimization search (or after updating each step of the CG method)
`wopt.dat`	Data required to take over the structure optimization history for a recalculation
`band_eigv`	Results of the band calculation (k-points, bands, eigenvalues)
`band_dedk`	Differentiation of bands
`vrho.dat1*`	Density/potential data
`wf.dat1*`	Wave function data

Depending on whether the program is executed for structure optimization or a band calculation the output may not include all of the files listed above. As mentioned above, some files must be used as input files in the recalculation.

For wave function data, there are two data-writing modes; one that writes all the data in a single file (`wf.dat1`) and one that writes data processed by each MPI rank in several files in parallel. In the latter case, only the basic parameters are stored in `wf.dat1` and wave function data is outputted by rank to separate files; for example, data processed by rank 3 is stored in a file named `wf.dat1.00003`.

3.5 Format of Parameter File: `fort.1`

The input parameters are given in the following format:

```
KEYWORD          value1  value2  ...
```

Although the default values are set for some of the undefined input parameters, the values of certain parameters must be specified. For example, KEYWORD must be specified. KEYWORD is not case-sensitive.

For example, assume the following list of values has been specified:

```
KEYWORD          value1  value2  / value3 ...
```

When the values are specified in this way, the program omits reading of the values following the symbol "/" in the same line. (This is a specification of Fortran.) It is recommended to always end each line with the "/" symbol.

3.5.1 Parameters

XCTYPE (Exchange-correlation Functional)

Specifies the exchange-correlation functional. Currently, the following exchange-correlation functionals are available:

```
XCTYPE  'LDAPZ81'
XCTYPE  'LDAPW92'
XCTYPE  'GGAPBE96' (or 'PBE' or 'PBE96')
XCTYPE  'PBEsol'
XCTYPE  'revPBE'
XCTYPE  'HSE' (or 'HSE06')
XCTYPE  'HF'
XCTYPE  'PBE0'
XCTYPE  'VDWDF'
```

SYSTYPE (Periodic/Isolated System Selection)

Specifies whether periodic-system or isolated-system calculations are performed.

```
SYSTYPE 0        (Three-dimensional periodic system)
SYSTYPE 1        (Molecule/isolated system (RSMOL))
```

To perform molecule/isolated-system calculations, input file `fort.2` is also required. Currently, the execution of RSMOL is supported by the double-precision-real version only. (Refer to 3.1.)

ISYM (Use of Symmetry)

Specifies whether the symmetry of the crystal is to be used. (ISYM is available only for periodic system calculations.) To use ISYM (i.e., ISYM=1), the file that describes the symmetry operations must also be specified.

```
ISYM    0 /                         (Uses no symmetry)
ISYM    1  'symmetry_file'          (Uses symmetry)
```

AX, A1, A2, A3 (Real Lattice Vectors)

Specify the unit cell. The following is an example of the unit cell for Si with a two-atom diamond structure.

```
AX        10.261             (Lattice constant in units of atoms)
A1        0.0  0.5  0.5      (x, y, z components of a1 vector)
A2        0.5  0.0  0.5      (x, y, z components of a2 vector)
A3        0.5  0.5  0.0      (x, y, z components of a3 vector)
```

NGRID (Real-space Grid Spacing)

Specifies how many sections that the space should be divided in the direction of the lattice vectors. This parameter is ignored in molecule-version (RSMOL) calculations.

```
NGRID   12  12  12
```

MD (Degree of Difference Equations)

Specifies the degree of the difference equations using the (2MD+1)-point formula.

```
MD      6
```

NBAND (Number of Bands)

Specifies the number of bands to calculate. In the case of the SCF calculations, convergence can be improved by setting the number of bands to approximately 10 percent more than the number of bands occupied by electrons.

```
NBAND   16
```

NSPIN (Spin Number)

Specifies the freedom of spin.

```
NSPIN   1       (Calculates electrons without spin)
NSPIN   2       (Calculates electrons with spin)
```

NDSPIN (Initial Spin Difference)

Specifies the initial value (≥ 0.0) of the difference in the number of electrons with spin. RSDFT executes the SCF calculations while keeping this difference as many times as specified by the next `NFIXED` parameter. If a negative value is specified, the mode reads the initial spin configuration of each atomic site from `fort.980`.

```
NDSPIN    1.0   (Calculates the SCF by setting difference in number of
          electrons between up and down to 1.0)
NSPIN   -1.0    (Reads the initial spin configuration from fort.980)
```

NFIXED (Number of Iterations to Keep the Initial Spin Difference)

RSDFT executes the SCF calculations while keeping the difference in the number of electrons with spin specified by NDSPIN for a set number of iterations.

```
NFIXED    10        (Keeps the difference in the number of electrons with spin
for 10 iterations of the SCF calculations)
```

NEXTE (Charge State)

Specifies the number of electrons to charge from outside. A positive number indicates a negative charge state.

```
NEXTE     1.0       (Calculates the charge state of −1, meaning that the
number of electrons is one more than the neutral state)
```

NK (Number of Grid Sections in the BZ)

Specifies how many sections (NK^3) to divide the BZ. If this parameter is specified, the next parameters mmm1 and mmm2 must be specified to indicate which grid points to use for the sampling.

```
NK        8         (Divides the BZ into 8³ grid sections, with coordinates
ranging from −4 to +4 given)
```

mmm1 (Coordinates of the Grid Point in the BZ to Start Sampling)

Specifies the coordinates of the grid point to start sampling after dividing the BZ into NK^3 grid sections. RSDFT interprets any value outside of the coordinate range in NK above as the specification of a value in the range from −NK/2 to +NK/2 based on the periodic boundary condition.

```
mmm1      5  5  5   (Coordinates of the grid point in the BZ to start sampling)
```

mmm2 (Interval of the Grid Points in the BZ for Sampling)

Specifies the interval of grid points to sample after dividing the BZ into NK^3 grids and starting sampling at the coordinates specified by mmm1.

```
mmm2      2  2  2   ( Sampling with an interval of two grid points
                     (at every other grid point) in the BZ )
```

EKBT (Temperature for the BZ Integration by Smearing)

Specifies the temperature to perform the BZ integration by smearing based on the Methfessel-Paxton met previous calculations is necessary to restart the calculations.hod.

```
EKBT     1.0d-5   (Hartree atomic units)
```

KINTEG (Delta Function Expansion)

Specifies the degree of Hermite polynomials used to expand the delta function in the BZ integration by smearing based on the Methfessel-Paxton method.

```
KINTEG  5
```

SWSCF (Enabling/Disabling Initial SCF Calculation)

Specifies whether to enable or disable the SCF calculations at the initial atomic coordinates (from fort.970).

```
SWSCF   1        (Enables the initial SCF calculation)
SWSCF   0        (Disables the initial SCF calculation)
```

DITER (Upper Limit of the Number of SCF Iteration Loops)

This parameter can be specified separately for the structure optimization and the band calculation.

```
DITER   100
```

NSWEEP (Upper Limit of Loops per Sweep Calculation)

Specifies the upper limit of the number of iterations in the sweep calculation, which is a kind of SCF calculation with a fixed initial potential executed by RSDFT to improve the initial wave functions.

```
NSWEEP  20
```

ICG (Wave Function Update Algorithm)

Currently RSDFT uses the Rayleigh quotient minimization based on the conjugate gradient (CG) method. The following options are currently available:

```
ICG      1          (CG method by Bylander-Kleinam-Lee)
ICG      2          (LOBPCG method)
```

IPC (Preprocessing of Wave Function Update Algorithm)

```
IPC      1          (Incomplete CG iterations)
ICG      2          (Tuned incomplete CG)
ICG      4          (Incomplete CG for thread parallel operation)
```

The following can be used as the preprocessing of the CG method:

MLOOP (Number of Incomplete CG Preprocessing Iterations)

Specifies the upper limit for the number of iterations in incomplete CG preprocessing. Empirically, a value of three is appropriate.

```
MLOOP    3          (Number of CG Iterations for preprocessing of CG
method)
```

NCG (Number of CG Iterations for Wave Function Update)

Empirically, it seems appropriate to set this to a value of two or three in view of the convergence and calculation time.

```
NCG      2
```

IMIX (Mixing of Density/Potential)

Specifies the method to produce an input by extrapolation from the density or potential obtained in previous iterations to achieve SCF convergence.

```
IMIX     0        (Update by density, simple mixing)
IMIX     1        (Update by potential, simple mixing)
IMIX     10       (Update by density, Pulay method)
IMIX     11       (Update by potential, Pulay method)
IMIX     20       (Update by density, Broyden method)
IMIX     21       (Update by potential, Broyden method)
```

MMIX (Mixing of Density/Potential)

Specifies how many past samples of data to use for the extrapolation.

```
MMIX     4        (Uses four past samples of density/potential data to
                extrapolate next input)
```

BETA (Mixing of Density/Potential)

Specifies the mixing rate of data generated by extrapolation to the current data. If BETA is less than 1.0, the specified value is determined as the final value for the next input. If BETA is set to 1.0, the mixing rate is adjusted during the calculation.

```
BETA     1.0      (Automatically adjusts mixing rate when BETA = 1.0)
```

SCFCONV (Tolerance for SCF Convergence)

Specifies the tolerance for the potential/density convergence. Normally, only the potential is used to make judgments. However, another option is to use both the potential and the density.

```
SCFCONV 1.d-15  1.d-15  (Judgment condition for potential/density
                               convergence)
```

The quantity used for this judgment is given by

$$\frac{1}{\Omega_{cell}}\int_{\Omega_{cell}}\left|f^{new}(\mathbf{r})-f^{old}(\mathbf{r})\right|d\mathbf{r} \tag{3.1}$$

ETOTCONV (Tolerance for SCF Convergence by Total energy)

Specifies the tolerance for SCF convergence by the error in total energy.

```
ETOTCONV        1.0d-12
```

FMAXCONV (Tolerance for SCF Convergence by Force)

Specifies the tolerance for SCF convergence by force. RSDFT calculates the Hellmann–Feynman force in the middle of the SCF iterations and terminates the SCF iteration process when the maximum value almost converges to a constant value.

```
FMAXCONV        1.0d-5
```

PP (Pseudopotential Format and File Name)

Describes the pseudopotential format and file name as many times as the number of elements provided in fort.970 in the order of the serial element number. For example, the case of SiC (with two elements) is described as:

```
PP      2       'Si_psv.dat'  (Data format and file name)
PP      2       'C_psv.dat'  (Data format and file name)
```

Currently RSDFT supports the following pseudopotential data formats:

```
PP      1       (TM format
                http://bohr.inesc-mn.pt/~jlm/pseudo.html)
PP      2       (PSV format)
PP      3       (YB format)
PP      4       (GTH/HGH format)
PP      5       (UPF format
        http://www.quantum-espresso.org/pseudopotentials)
PP      102      PSV ultrasoft pseudopotential)
```

SWOPT (Atomic Structure Optimization)

Controls the atomic structure optimization calculations. The wopt.dat generated at the end of the previous calculations is necessary to restart the calculations.

```
SWOPT   0       (Disables structure optimization)
SWOPT   1       (Enables structure optimization)
SWOPT   2       (Restarts structure optimization calculations. wopt.dat is
              required.)
```

ATOMOPT1 (Atomic Structure Optimization)

Controls the atomic structure optimization calculations based on the conjugate gradient (CG) method. It specifies the upper limit of the number of CG iterations, the number of linear search trials in each CG, and the CG refresh timing.

```
ATOMOPT1  10  6  5 (Number of CG iterations, number of linear search steps, and
                    CG refresh timing)
```

ATOMOPT2 (Atomic Structure Optimization)

Controls the atomic structure optimization calculations based on the conjugate gradient (CG) method. It specifies the upper limit of the atom transfer distance, the judgment condition for the energy convergence, the judgment condition for the force convergence, and the judgment condition for the linear search convergence.

```
ATOMOPT2  0.5  1.d-10  5.d-4  1.d-1 (Maximum allowable atom transfer,
judgment condition for energy convergence, judgment condition for force
convergence, and judgment condition for linear search convergence)
```

ATOMOPT3 (Number of SCF Iterations during Atomic Structure Optimization)

Specifies the upper limit of the number of SCF iterations in the SCF calculations during an atomic structure optimization.

```
ATOMOPT3        100
```

TIM (Constraint Condition in Atomic Structure Optimization)

Describes the elements of the 3×3 matrix that represents the constraint conditions for force in the three lines following this keyword. This constraint matrix must be described as the maximum value of the constraint condition number parameter in the fourth column of the atomic coordinate file (fort.970). If this parameter is omitted, RSDFT specifies the unit matrix. The actual force to be applied to move atoms is the force calculated per atom multiplied by the constraint matrices (or matrix) specified here. The following is an example of how to specify TIM so that only the z component is changed.

```
TIM
0.0  0.0  0.0      (Cxx, Cxy, and Cxz elements of constraint matrix C)
0.0  0.0  0.0      (Cyx, Cyy, and Cyz elements of constraint matrix C)
0.0  0.0  1.0      (Czx, Czy, and Czz elements of constraint matrix C)
```

IC (File I/O Control)

Specifies whether to read wave function and density/potential data to restart the calculations or to perform band calculations.

`IC`	`0`	(Reads no data)
`IC`	`1`	(Reads wave function data only)
`IC`	`2`	(Reads density/potential data only)
`IC`	`3`	(Reads both data)

`OC (File I/O Control)`

Specifies whether to write wave function and density/potential data.

`OC`	`0`	(Writes no data)
`OC`	`1`	(Writes wave function data only)
`OC`	`2`	(Writes density/potential data only)
`OC`	`3`	(Writes both data)
`OC`	`4`	(Writes only wave function data in single precision)
`OC`	`5`	(Writes density, potential, and single-precision wave function data)

`OC2 (File I/O Control)`

Specifies how many SCF iterations to execute before writing data.

`OC2`	`100`	(Writes data once in every 100 iterations)

`IOCTRL (File I/O Control)`

Specifies whether to write wave function data for all ranks collectively as rank 0 or to write wave function data for each rank separately in parallel calculations. If data for each rank is written separately, the data is written to a separate file with a file name that includes a five-digit rank number, such as wf.dat1.00000.

```
IOCTRL   0            (Writes all data collectively as rank 0)
IOCTRL   3            (Writes data for each rank separately)
```

PROCS (Number of MPI Parallel Processes)

Specifies the number of parallel processes to perform the grid, band, k-point, and spin calculations. The product of all digits must match the number of MPI processes specified during program execution.

```
PROCS     2   2   2   1   1   1   (Parallelizes space into 2 × 2 × 2 processes)
```

ETLIMIT (Upper Limit of Elapsed Time)

Specifies the upper limit of the elapsed time. RSDFT completes the calculations after writing data such as wave function data when the set time has elapsed.

```
ETLIMIT 86400.0  (Sets elapsed time to 24 hours = 86,400 seconds)
```

SWBAND (Band Calculation Control)

Specifies whether to enable or disable band calculations.

```
SWBAND   0            (Disables band calculation)
SWBAND   1            (Enables band calculation)
```

BAND (Band Calculation Parameter)

Specifies the coordinates of the k-points and the number of divisions of the sections in the lines following the line that defines the keyword and parameters. In particular, in the line beginning with the keyword, the number of sections in which to draw bands, the number of bands to use in the calculations, the number of bands to retrieve as a result, the judgment condition for convergence by a constant, and the upper limit of the number of SCF iterations during band calculation must be specified. Then, in the next three lines, the coordinates of the k-points in each section are described as many as the number of sections on the basis of the reciprocal lattice vectors, where the values are given by

$$\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3 \tag{3.2}$$

Finally, in the last line, the number of divisions of each section is specified as many as the number of sections. Below is an example for four sections.

```
BAND    3  24  20  1.d-7  100
0.0  0.0  0.0  0.5
0.0  0.0  0.5  0.5
0.0  0.5  0.5  0.5
10  10  10  10
```

3.6 Format of the Atomic Coordinate File: fort.970

Specifies the numbers of elements and the number of atoms in the unit cell, the atomic numbers, and the initial atomic coordinates. Although this file can also describe information in the unit cell (lattice vectors), the information in fort.1 is given priority if there is a discrepancy. The following is an example of the unit cell of Si with a two-atom diamond structure.

```
AX  10.261
A1  0.0  0.5  0.5
A2  0.5  0.0  0.5
A3  0.5  0.5  0.0
AA
1  2  14            (Number of elements, number of atoms, atomic number ①, atomic number ②,...)
1  0.00  0.00  0.00  1    (Element, coordinate, coordinate, coordinate, constraint condition)
1  0.25  0.25  0.25  1    (Element, coordinate, coordinate, coordinate, constraint condition)
```

When this information is described as shown above, RSDFT interprets that the atomic coordinates are in a lattice vector representation.

```
AX  10.261
A1  0.0  0.5  0.5
A2  0.5  0.0  0.5
A3  0.5  0.5  0.0
XYZ
1  2  14            (Number of elements, number of atoms, atomic number ①, atomic number ②, ...)
1  0.00000  0.00000  0.00000  1
1  2.56525  2.56525  2.56525  1
```

When the information is described as shown above, RSDFT interprets that the atomic coordinates are in the XYZ representation.

3.7 Format of the Initial Spin Configuration File: fort.980

Assuming that each atom is given a serial number in the order that it is written in the atomic coordinate file, the initial spin is specified as:

```
 1   5  1.00      (Sets difference in number of electrons with spin to 1.00 for 1–5th atom sites)
 6   6  0.50      (Sets difference in number of electrons to 0.50 for 6th atom site)
11   12  1.00     (Sets difference in number of electrons to 1.00 for 11–12th atom sites)
```

The initial electron density is provided so that the difference in the number of spin is reproduced.

3.8 Symmetry Operation File

Provides data in the following format. In fort.1, this file can be given any file name.

`nsym nnp` (Number of symmetry operations, inverse of translation)

R_{11} R_{12} R_{13} R_{21} R_{22} R_{23} R_{31} R_{32} R_{33} t_1 t_2 t_3 (Symmetry operation matrix, translation vector)

…

The symmetry operation matrix and translation vector data should be given in the lattice-coordinate representation. In other words, when the position vector is

$$\begin{aligned}\mathbf{r} &= x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z \\ &= \alpha\mathbf{a}_1 + \beta\mathbf{a}_2 + \gamma\mathbf{a}_3\end{aligned} \tag{3.3}$$

the transformation of (α,β,γ) is given by

$$\begin{pmatrix}\alpha' \\ \beta' \\ \gamma'\end{pmatrix} = \begin{pmatrix}R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33}\end{pmatrix}\begin{pmatrix}\alpha \\ \beta \\ \gamma\end{pmatrix} + \frac{1}{\mathrm{nnp}}\begin{pmatrix}t_1 \\ t_2 \\ t_3\end{pmatrix} \tag{3.4}$$

3.9 Molecule/Isolated System Calculation (RSMOL) Parameters: fort.2

RSMOL and RSSOL (periodic system) differ in how the calculation domain and grid are specified. RSMOL requires the following additional parameters:

`1`	(Spherical simulation box is used)
`0.30  20.0`	(Grid spacing is 0.3 bohr and a radius of SimBox is 20 bohrs)
`1`	(Uses grid division in consideration of load balancing)

If the "grid division in consideration of load balancing" parameter in the third line is set to `2`, RSDFT tries to divide the grid so that the load balance is further improved, despite the increase in the communication cost.

Note that, in the case of RSMOL, the grid resolution is determined only by the grid spacing specified in `fort.2`. Additionally, the size of the simulation box also affects the calculation results. You must care of the convergence of the results with respect to these two parameters.

4 Utility Programs

This chapter describes the function of each program found in the `utility/` directory.

4.1 Creation of Atomic Coordinates

sol_conf

This program creates a rectangular supercell with a diamond structure. It reads three integers (`nc1, nc2, nc3`) from the standard input and writes the atomic coordinates of a supercell with `8*nc1*nc2*nc3` atoms to `fort.970`. Below is an example of the compilation and execution process of the program.

```
[iwata@kaki utility]$ ifort sol_conf.f90
[iwata@kaki utility]$ ./a.out
 input size of the unit cell : nc1,nc2,nc3=
 ( # of atoms is 8*nc1*nc2*nc3 )
11 11 11
 # of nodes =          1
 # of atoms =      10648
 # of grid points =     5451776
 # of eigenstates      23426
 memory estimation (GB) =   1903.07653808594
```

4.2 Drawing of Band Diagram

band2gp

When a band calculation is executed, RSDFT writes k-point and eigenvalue data to the file named `band_eigv`. This program creates the data and script for gnuplot from this file. Below is an example of the compilation and execution process of the program.

```
> ls
band_eigv
> ifort band2gp.f90
> ./a.out
> ls
> plot_band  fort.2001  fort.2002 .....
> gnuplot
gnuplot> load 'plot band'
```

4.3 Visualization of Atomic Coordinates, Density/Potential, and Wave Functions

cubegen_simple

This program reads the atomic coordinate file, which is a file format that also contains information about the unit cell (lattice vectors), from the standard input to generate a cube-format file. The file name of this output file is `tmp.cube`. The cube file can be read into drawing software such as VMD and VESTA to visualize the atomic coordinates. Below is an example of the execution process of the program.

```
> ifort cubegen_simple.f90
> ./a.out < fort.970
> ls
> fort.970 tmp.cube
```

cubegen_vrho

This program generates cube files that contain drawing data for density, potential, and spin density from two files: fort.970 and vrho.dat1. The former also contains information about the unit cell (lattice vectors), while the latter is an output of RSDFT that contains density and potential data. Below is an example of the execution process of the program.

```
> ifort cubegen_vrho.f90
> ls
fort.970 vrho.dat1
> ./a.out
```

When the freedom of spin is not considered, the output is

```
> ls
rho_1.cub vloc_1.cub
```

When the freedom of spin is considered, the output is

```
> ls
dspin_1.cub rho_1.cub rho_2.cub vloc_1.cub vloc_2.cub
```

By reading these files into software such as VMD and VESTA, the isosurfaces and contours of density and potential can be drawn over the atomic coordinates.

cubegen_wf

This program generates cube files that also contain drawing data for wave functions from two files: fort.970 and wf.dat1. The former contains information about the unit cell, while the latter is the wave function data file output with divided writing disabled (IOCTRL = 1). As shown below, cubegen_wf requires a dedicated input.

```
R        2        / Real ('r' or 'R') or complex ('c' or 'C'), iflag_abs
wf.dat1           / Wave function data file name
1                 / Number of sample k-points (Nbzsm)
1                 / Freedom of spin (Nspin)
4                 / Number of samples of wave function data to generate
1 1 1             / n1, k1, s1 (Specification of band, k-point, and spin;
2 1 1             / n2, k2, s2 This specification is given in 4 lines here
3 1 1             / n3, k3, s3 as number of samples of data is 4)
4 1 1             / n4, k4, s4
```

If iflag_abs = 0, then RSDFT outputs data, including the signs of wave functions (supported by the real-value version only). RSDFT outputs the absolute values if iflag_abs = 1 and the squares of absolute values if iflag_abs = 2 as drawing data. Below is an example of the execution process of the program.

```
> ls
fort.970  input_cubgen_wf  wf.dat1
# ./a.out < input_cubgen_wf
# ls
wf_00001_001_1.cub  wf_00002_001_1.cub …
```

(The number portion after wf_ represents band_k_point_spin.)

cubegen_wf3

This program generates cube files that contain drawing data for wave functions from fort.970, which contains information about the unit cell, and the wave function data (IOCTRL = 3) output with division writing enabled. When executing RSDFT, this program must be executed as a parallel job with the number of specified parallel processes. This program requires a dedicated input file named fort.3. The contents of this file are almost the same as cubegen_wf, except for the one line added to the end of the file to indicate the number of parallel processes.

```
R        2            / Real ('r' or 'R') or complex ('c' or 'C'), iflag_abs
wf.dat1               / Wave function data file name
1                     / Number of sample k-points (Nbzsm)
1                     / Freedom of spin (Nspin)
4                     / Number of samples of wave function data to generate
1 1 1                 / n1, k1, s1 (Specification of band, k-point, and spin;
2 1 1                 / n2, k2, s2 This specification is given in 4 lines here
3 1 1                 / n3, k3, s3 as number of samples of data is 4)
4  1  1               / n4, k4, s4
PROCS    2 2 2 1 1 1/ Specify same keyword and parallel number
                              as those used when executing RSDFT
```

The output files are exactly the same as those of cubegen_wf. Below is an example of the execution process of the program.

```
# ls
fort.3  fort.970  wf.dat1  wf.dat1.00000  wf.dat1.00001 …
# mpirun -np 8 ./cubegen_wf3
# ls
wf_00001_001_1.cub  wf_00002_001_1.cub …
(The number portion after wf_ represents band_k_point_spin.)
```

5 Known Discrepancies

- In the oblique coordinates of fcc or bcc lattice, finite-difference formula seems to break the symmetry at the gamma point. Therefore, denser grid points are necessary to recover the symmetry of fcc or bcc lattice.