物質科学のための計算数理 II
Numerical Analysis for Material Science II

11th: Density Functional Theory (4)
Dec. 21 (Fri)

Lecturer: Mitsuaki Kawamura (河村光晶)

Schedule (This semester W1, W2)

1. Sep. 28 (Fri) Guidance Y
2. Oct. 5 (Fri) Monte Carlo method O
3. Oct. 12 (Fri) Monte Carlo method O
4. Oct. 19 (Fri) Monte Carlo method O
5. Oct. 26 (Fri) Exact diagonalization Y
6. Nov. 2 (Fri) Exact diagonalization Y
7. Nov. 9 (Fri) Molecular dynamics O (1st report problem will be announced.)
8. Nov. 30 (Fri) Density functional theory K
9. Dec. 7 (Fri) Density functional theory K
10. Dec. 14 (Fri) Density functional theory K
11. Dec. 21 (Fri) Density functional theory K
12. Dec. 25 (Tue) Density functional theory K (遠隔講義室)
13. Jan. 11 (Fri) (2nd)Report problem K

※ Lecturers: Y … Yamaji, K … Kawamura, O… Ohgoe

Schedule in this section (DFT)

1. Nov. 30 (Fri) Standard DFT code
   - First-principles calculation and Density functional theory (Lecture)
   - One-body Schrödinger eq. for periodic system and Bloch theorem (L)
   - Numerical solution of Kohn-Sham (one-body Schrödinger) eq. (L)
   - Hands-on DFT code (Tutorial)
   - Version control system : Git (T)
2. Dec. 7 (Fri) Kohn-Sham eq.
   - Plane-wave basis and Pseudopotentials (L)
   - Iterative eigenvalue solution method (L & T)
3. Dec. 14 (Fri) Self-Consistent loop
   - Hartree potential (Poisson eq.), Atomic potential, XC potential
   - Update (Broyden's method)
   - Visualization of grid data (T)
4. Dec. 21 (Fri) Total Energy
   - Total energy
   - Brillouin-zone integral (Tetrahedron method)
   - Coulomb potential for periodic point charge (Ewald sum)
5. Dec. 25 (Tue) Advanced subjects for productive calculation (遠隔講義室)
   - Generalized gradient correction
   - Non-local pseudopotentials (Norm-conserving, ultrasoft, PAW)
   - Procedure
6. Jan. 11 (Fri) (2nd) Report problem, Question time

Today's Schedule

- Total energy
  - Hartree term
  - Exchange correlation term
- Brillouin-zone integration
  - Basics
  - Smearing method
  - Tetrahedron method and its improvement
- Fermi surface plot

Total energy functional for DFT

$$E_{tot} = E[\rho] + \frac{1}{2}\sum_{R,R'}^{N_c}\sum_{\boldsymbol{\tau},\boldsymbol{\tau}'}^{N} \frac{Z_{\boldsymbol{\tau}} Z_{\boldsymbol{\tau}'}(1-\delta_{RR'}\delta_{\boldsymbol{\tau}\boldsymbol{\tau}'})}{|\boldsymbol{\tau}+\boldsymbol{R}-\boldsymbol{\tau}'-\boldsymbol{R}'|}$$

$$E[\rho] = \int d^3r \rho(\boldsymbol{r})\, v(\boldsymbol{r}) + E_{univ}[\rho]$$

$$E_{univ}[\rho] = T_{KS}[\rho] + \frac{1}{2}\iint d^3r d^3r' \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + E_{XC}[\rho]$$

$$T_{KS}[\rho] = N_c \int_{BZ} \frac{d^3k}{V_{BZ}} \sum_n \int d^3r \varphi^*_{n\boldsymbol{k}}(r)\left(-\frac{\boldsymbol{\nabla}^2}{2}\right)\varphi_{n\boldsymbol{k}}(r)$$

$$= N_c \int_{BZ} \frac{d^3k}{V_{BZ}} \sum_n \sum_{\boldsymbol{G}} \frac{|\boldsymbol{k}+\boldsymbol{G}|^2}{2} |\tilde{u}_{n\boldsymbol{k}}(\boldsymbol{G})|^2$$

$$\varphi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{N_C} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$u_{n\boldsymbol{k}}(\boldsymbol{r}) = \sum_G \tilde{u}_{n\boldsymbol{k}}(\boldsymbol{G}) \frac{e^{i\boldsymbol{G}\cdot\boldsymbol{r}}}{\sqrt{V_{uc}}}$$

Local density approximation

$$E_{XC}[\rho] = \int d^3r \rho(r)\varepsilon_{XC}\big(\rho(r)\big) = N_c \int_{uc} d^3r r\rho(r)\varepsilon_{XC}\big(\rho(r)\big)$$

Tutorial for total energy

```
$ cd ~/pwdft/
$ git checkout master
$ git pull
$ make clean; make
$ cd sample/Al/
$ ../../src/pwdft.x < scf.in
```

```
Energy per u.c. [eV]
     Kinetic energy :     22.571740309226847
     Hartree energy :    0.1095435926455650 1
     rho*V :     14.630190122503379
       Ewald eta [Bohr^-1] :     1.4221682587100493
       Ewald grid (G) :       25      25      25
       Ewald grid (R) :        2       2       2
     Eward energy :    -73.366857049902464
     XC energy :    -21.802851254893593
     Total energy :    -57.858234280420255
```

```
$ bash vol.sh
```

Hartree and atomic potential

energy.F90

$$\frac{1}{2}\iint d^3r d^3r' \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} = \frac{1}{2}\sum_{\boldsymbol{G},\boldsymbol{G}'} \tilde{\rho}(\boldsymbol{G})\tilde{\rho}(\boldsymbol{G}') \iint d^3r d^3r' \frac{e^{i\boldsymbol{G}\cdot\boldsymbol{r}} e^{i\boldsymbol{G}'\cdot\boldsymbol{r}'}}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

$$= \frac{1}{2}\sum_{\boldsymbol{G},\boldsymbol{G}'} \tilde{\rho}(\boldsymbol{G})\tilde{\rho}(\boldsymbol{G}') \int d^3r' e^{i(\boldsymbol{G}+\boldsymbol{G}')\cdot\boldsymbol{r}'} \int d^3r \frac{e^{i\boldsymbol{G}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

$$= \frac{N_c V_{uc}}{2}\sum_{\boldsymbol{G}} \tilde{\rho}(\boldsymbol{G})\tilde{\rho}(-\boldsymbol{G}) \frac{4\pi}{|\boldsymbol{G}|^2} = \frac{N_c V_{uc}}{2}\sum_{\boldsymbol{G}} |\tilde{\rho}(\boldsymbol{G})|^2 \frac{4\pi}{|\boldsymbol{G}|^2}$$

$$\lim_{\boldsymbol{G}\to 0} \frac{N_c V_{uc}}{2} \frac{4\pi}{|\boldsymbol{G}|^2} \left(\frac{N}{V_{uc}}\right)^2$$

Atomic potential term

$$\int d^3r \rho(\boldsymbol{r})\, v(\boldsymbol{r}) = \sum_{\boldsymbol{G},\boldsymbol{G}'} \tilde{\rho}(\boldsymbol{G})\tilde{v}(\boldsymbol{G}') \int d^3r e^{i\boldsymbol{G}\cdot\boldsymbol{r}} e^{i\boldsymbol{G}'\cdot\boldsymbol{r}'} = N_c V_{uc} \sum_{\boldsymbol{G},\boldsymbol{G}'} \tilde{\rho}(\boldsymbol{G})\tilde{v}(-\boldsymbol{G})$$

Compensating divergent term

$$-\lim_{\boldsymbol{G}\to 0} N_c V_{uc} \frac{4\pi}{|\boldsymbol{G}|^2} \left(\frac{N}{V_{uc}}\right)^2$$

Ion–ion Coulomb repulsion

$$\frac{1}{2}\sum_{R,R'}^{N_c}\sum_{\tau,\tau'}^{N}\frac{Z_\tau Z_{\tau'}(1-\delta_{RR'}\delta_{\tau\tau'})}{|\tau+R-\tau'-R'|}=\frac{N_c}{2}\sum_{R}^{N_c}\sum_{\tau,\tau'}^{N}\frac{Z_\tau Z_{\tau'}(1-\delta_{R0}\delta_{\tau\tau'})}{|\tau-\tau'+R|}$$

$$=\frac{N_c}{2}\sum_{\tau,\tau'}^{N}Z_\tau Z_{\tau'}\sum_{R}^{N_c}\frac{1-\delta_{R0}\delta_{\tau\tau'}}{|\tau-\tau'+R|}$$

$$\int d^3r\,\frac{e^{-iG\cdot r}}{|r|}$$

$$\sum_{R}^{N_c}\frac{1}{|r+R|}=\sum_{G}e^{iG\cdot r}\int_{uc}\frac{d^3r'}{V_{uc}}e^{-iG\cdot r'}\sum_{R}^{N_c}\frac{1}{|r'+R|}=\sum_{G}e^{iG\cdot r}\frac{4\pi}{V_{uc}|G|^2}$$

$$=\frac{N_c}{2}\sum_{\tau,\tau'}^{N}Z_\tau Z_{\tau'}\left(\sum_{G}e^{iG\cdot(\tau-\tau')}\frac{4\pi}{V_{uc}|G|^2}-\sum_{R}^{N_c}\frac{\delta_{R0}\delta_{\tau\tau'}}{|\tau-\tau'+R|}\right)$$

$$\lim_{G\to 0}\frac{N_cV_{uc}}{2}\frac{4\pi}{|G|^2}\left(\frac{N}{V_{uc}}\right)^2$$

Slow decay in sum $\sum_{R}\frac{1}{|R|}$ $\sum_{G}\frac{e^{iG\cdot r}}{|G|^2}$

Ewald's method (1)

$$\frac{1}{|\boldsymbol{r}+\boldsymbol{R}|}=\frac{2}{\sqrt{\pi}}\int_0^\infty dx e^{-|\boldsymbol{r}+\boldsymbol{R}|^2x^2}$$

$$\sum_{\boldsymbol{R}}^{N_c} e^{-|\boldsymbol{r}+\boldsymbol{R}|^2x^2}=\sum_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}\int_{uc}\frac{d^3r'}{V_{uc}}e^{-i\boldsymbol{G}\cdot\boldsymbol{r}'}\sum_{\boldsymbol{R}}^{N_c} e^{-|\boldsymbol{r}'+\boldsymbol{R}|^2x^2}=\sum_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}\frac{\pi^{\frac{3}{2}}e^{-\frac{|\boldsymbol{G}|^2}{4x^2}}}{V_{uc}x^3}$$

$$\frac{N_c}{2}\sum_{\boldsymbol{\tau},\boldsymbol{\tau}'}^{N} Z_{\boldsymbol{\tau}}Z_{\boldsymbol{\tau}'}\sum_{R}^{N_c}\frac{1-\delta_{R\boldsymbol{0}}\delta_{\boldsymbol{\tau}\boldsymbol{\tau}'}}{|\boldsymbol{\tau}-\boldsymbol{\tau}'+\boldsymbol{R}|}$$

$$=\frac{N_c}{2}\sum_{\boldsymbol{\tau},\boldsymbol{\tau}'}^{N} Z_{\boldsymbol{\tau}}Z_{\boldsymbol{\tau}'}\sum_{R}^{N_c}\frac{2}{\sqrt{\pi}}\left(\int_{\eta}^{\infty} dx e^{-|\boldsymbol{\tau}-\boldsymbol{\tau}'+\boldsymbol{R}|^2x^2}-\delta_{R\boldsymbol{0}}\delta_{\boldsymbol{\tau}\boldsymbol{\tau}'}\int_0^{\infty}dx\right)$$

$$+\frac{N_c}{2}\sum_{\boldsymbol{\tau},\boldsymbol{\tau}'}^{N} Z_{\boldsymbol{\tau}}Z_{\boldsymbol{\tau}'}\sum_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot(\boldsymbol{\tau}-\boldsymbol{\tau}')}\frac{2\pi}{V_{uc}}\int_0^{\eta}\frac{dx}{x^3}e^{-\frac{|\boldsymbol{G}|^2}{4x^2}}$$

$$\cos\left(\boldsymbol{G}\cdot(\boldsymbol{\tau}-\boldsymbol{\tau}')\right)$$

$$\frac{2e^{-\frac{|\boldsymbol{G}|^2}{4\eta^2}}}{|\boldsymbol{G}|^2}$$

Ewald's method (2)

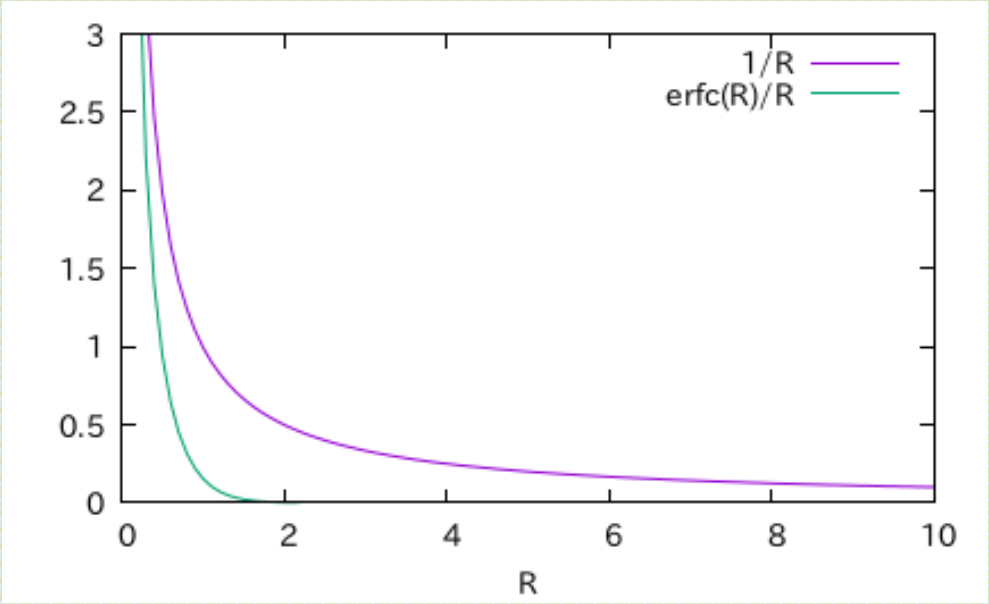
$$= \frac{N_c}{2}\sum_{\boldsymbol{\tau},\boldsymbol{\tau}'}^{N_S} Z_{\boldsymbol{\tau}} Z_{\boldsymbol{\tau}'} \sum_{R}^{N_c} (1-\delta_{R\mathbf{0}}\delta_{\boldsymbol{\tau}\boldsymbol{\tau}'}) \frac{2}{\sqrt{\pi}} \int_{\eta}^{\infty} dx e^{-|\boldsymbol{\tau}-\boldsymbol{\tau}'+\boldsymbol{R}|^2 x^2}$$

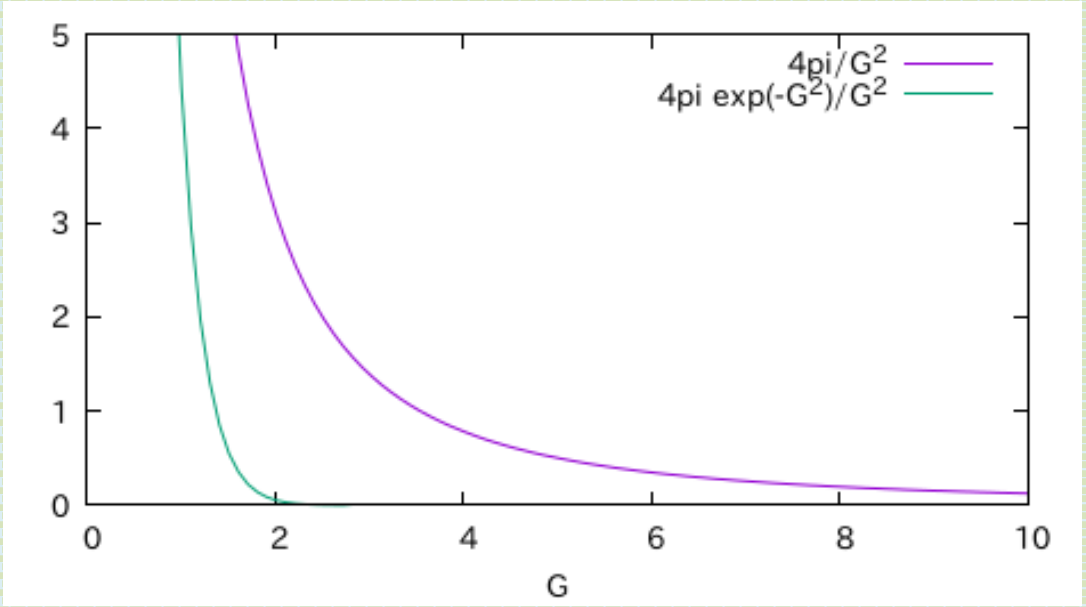
Complementary error function

$$\frac{\mathrm{erfc}(|\boldsymbol{\tau}-\boldsymbol{\tau}'+\boldsymbol{R}|\eta)}{|\boldsymbol{\tau}-\boldsymbol{\tau}'+\boldsymbol{R}|}$$

$$-\frac{N_c}{2}\sum_{\boldsymbol{\tau}}^{N} Z_{\boldsymbol{\tau}}^2 \frac{2}{\sqrt{\pi}} \int_{0}^{\eta} dx \qquad -N_c \sum_{\boldsymbol{\tau}}^{N} \frac{\eta Z_{\boldsymbol{\tau}}^2}{\sqrt{\pi}}$$

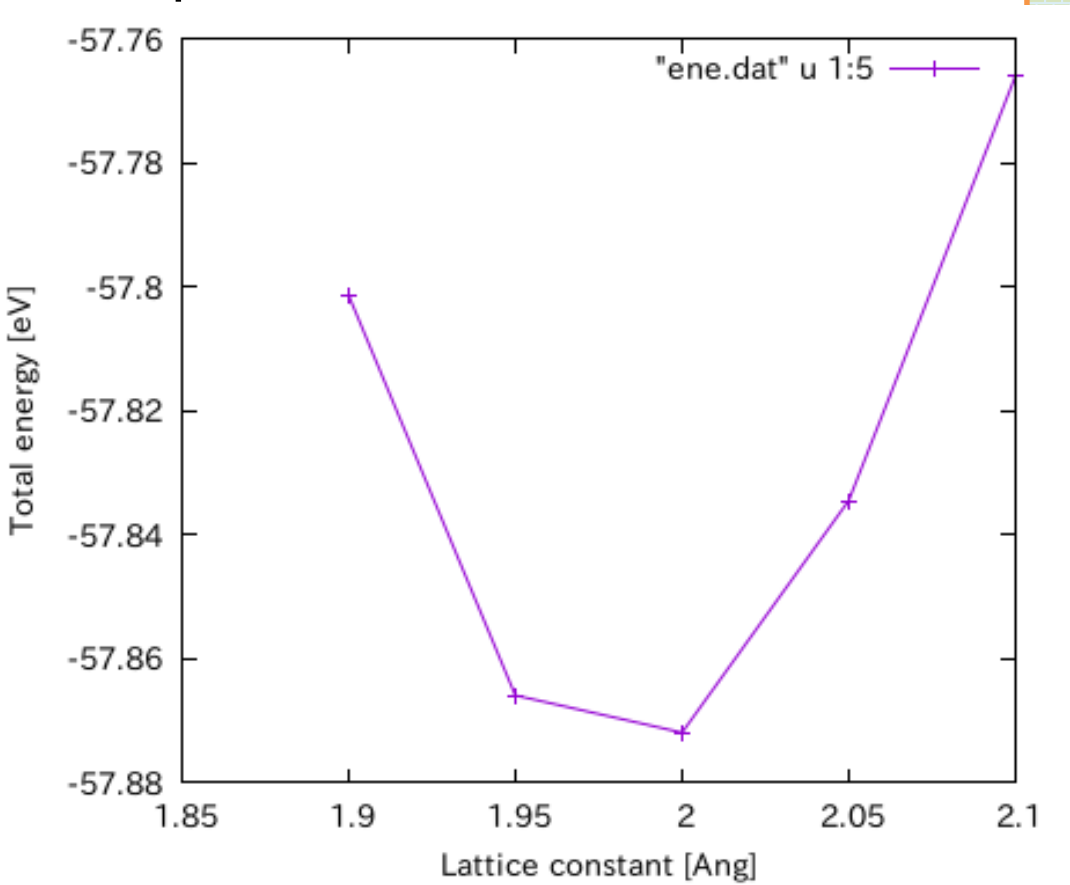
$$+\frac{N_c}{2}\sum_{\boldsymbol{\tau},\boldsymbol{\tau}'}^{N} Z_{\boldsymbol{\tau}} Z_{\boldsymbol{\tau}'} \sum_{\boldsymbol{G}\neq\mathbf{0}} \cos\left(\boldsymbol{G}\cdot(\boldsymbol{\tau}-\boldsymbol{\tau}')\right) \frac{4\pi e^{-\frac{|\boldsymbol{G}|^2}{4\eta^2}}}{V_{uc}|\boldsymbol{G}|^2} - \frac{N_c}{2}\frac{\pi N^2}{V_{uc}\eta^2} + \lim_{\boldsymbol{G}\to 0} \frac{N_c V_{uc}}{2} \frac{4\pi}{|\boldsymbol{G}|^2} \left(\frac{N}{V_{uc}}\right)^2$$





Optimize lattice constant

```
($ bash vol.sh)
$ grep "Total energy" scf*.out | ¥
sed -e 's/scf//g' -e 's/.out://g' > ene.dat
$ gnuplot
gnuplot> set xlabel "Lattice constant [Ang]"
gnuplot> set ylabel "Total energy [eV]"
gnuplot> plot "ene.dat" u 1:5 w lp
```



Brillouin-zone integration

$$\rho(r) = \sum_{\boldsymbol{k}} \sum_{n} |\varphi_{n\boldsymbol{k}}(r)|^2 \theta(\varepsilon_F - \varepsilon_{nk})$$

Born-von Karman's boundary condition : $\varphi_{n\boldsymbol{k}}(r + L) = \varphi_{n\boldsymbol{k}}(r) : L \to \infty$

The size of each state in the reciprocal space : $\left(\frac{2\pi}{L}\right)^3 = \frac{(2\pi)^3}{N_c V_{uc}}$

$$\sum_{\boldsymbol{k}} \cdots = \int_{BZ} \frac{d^3k}{(2\pi)^3/(N_c V_{uc})} \cdots = N_c \int_{BZ} \frac{d^3k}{V_{BZ}} \cdots$$

$$V_{uc} = |(\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_3| \qquad \frac{(2\pi)^3}{V_{uc}} \equiv V_{BZ} = |(\boldsymbol{b}_1 \times \boldsymbol{b}_2) \cdot \boldsymbol{b}_3|$$

$$\rho(r) = N_c \int_{BZ} \frac{d^3k}{V_{BZ}} \sum_{n} |\varphi_{n\boldsymbol{k}}(r)|^2 \theta(\varepsilon_F - \varepsilon_{nk}) = \int_{BZ} \frac{d^3k}{V_{BZ}} \sum_{n} |u_{n\boldsymbol{k}}(r)|^2 \theta(\varepsilon_F - \varepsilon_{nk})$$

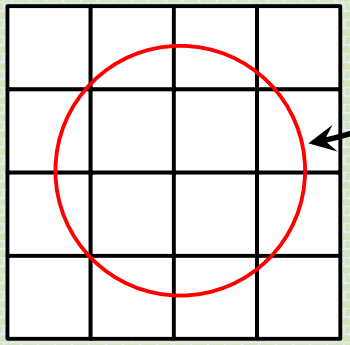
$\boldsymbol{k}$–integration with $\theta(\varepsilon_k)$ or $\delta(\varepsilon_k)$

Charge density

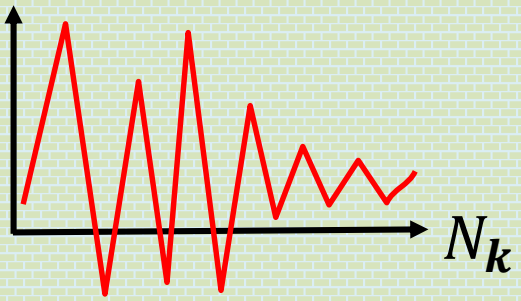
$$\rho(r) = \int_{BZ} \frac{d^3k}{V_{BZ}} \sum_n |u_{n\boldsymbol{k}}(r)|^2 \theta(\varepsilon_F - \varepsilon_{nk})$$

Density of states

$$D(\varepsilon) = \int_{BZ} \frac{d^3k}{V_{BZ}} \sum_n \delta(\varepsilon - \varepsilon_{nk})$$



Using $\theta(\varepsilon_F - \varepsilon_{nk})$ as is



Too many k points are required.

Broadening

M. Methfessel, A. T. Paxton, Phys. Rev. B 40, 3616 (1989).

Replace $\theta(\varepsilon_F - \varepsilon_{nk})$ with a smeared function such as the error function.

Tetrahedron

O. Jepsen and O. K. Andersen, Solid State Commun. 9, 1763 (1971).

Why we need to reduce k-points?

E.g. 1 DFT calculation of crystals with plane wave and pseudopotencial.

$v_{KS}(\boldsymbol{r})u_{n\boldsymbol{k}}(\boldsymbol{r})$ (for all orbitals) $\mathrm{O}(N_{\boldsymbol{k}} \times N_b \times N_{PW} \log N_{PW})$

Subspace diagonalization $\mathrm{O}\left(N_{\boldsymbol{k}} \times N_b^3\right)$

Update $\tilde{u}_{n\boldsymbol{k}}(\boldsymbol{G})$ $\mathrm{O}\left(N_{\boldsymbol{k}} \times N_b^2 \times N_{PW}\right)$

E.g. 2 Hartree-Fock, hybrid DFT, TC, GW

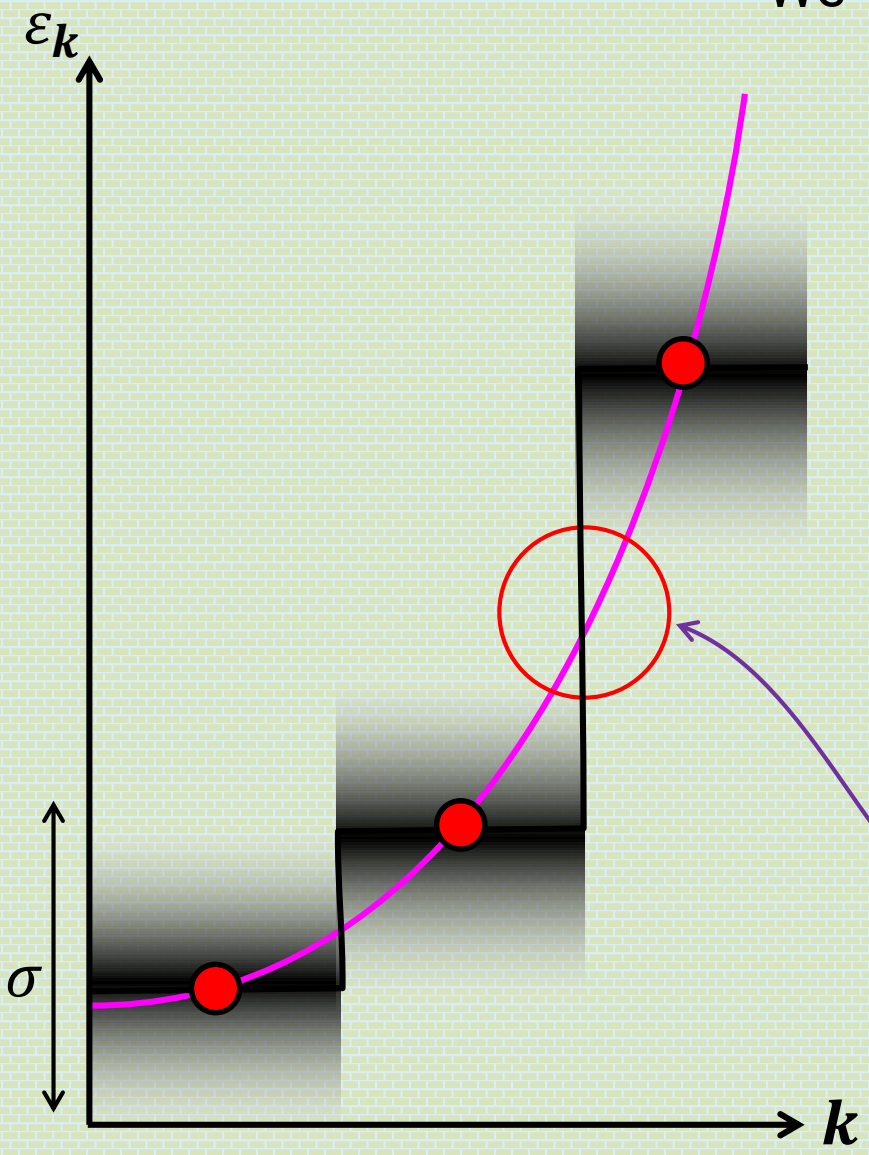
$\hat{v}_{Fock}u_{n\boldsymbol{k}}(\boldsymbol{r})$ (for all orbitals) $\mathrm{O}\left(N_{\boldsymbol{k}}^2 \times N_b^2 \times N_{PW} \log N_{PW}\right)$

※ N_b ～ The number of electrons

The reduction of k-points without loss of accuracy is the best way for efficient calculation.

Broadening method

We can calculate only on discrete k–points.



True band structure

Replace $\delta(x)$ with smeared function such as (Hermite) Gaussian.

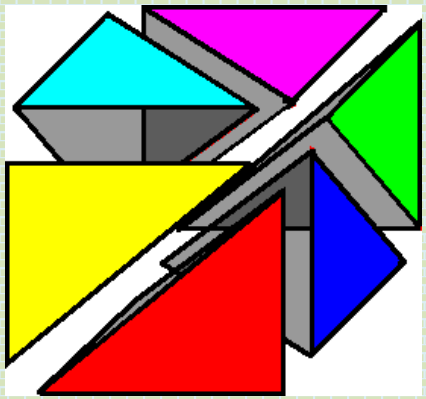
$$\delta(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\,4^n\sqrt{\pi}} H_{2n}\left(\frac{x}{\sigma}\right) e^{-x^2/\sigma^2}$$

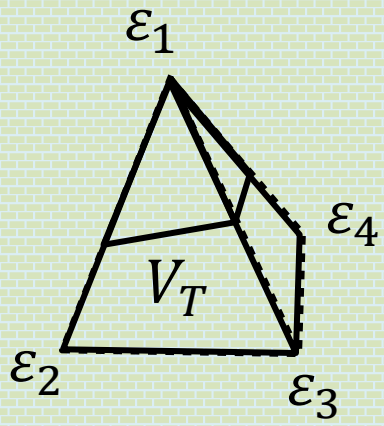
M. Methfessel and A. T. Paxton, Phys. Rev. B 40, 3616 (1989).

This method becomes worse when smeared function not cover all energy range.

Interpolation method

`libtetrabz_occ_main@libtetrabz/libtetrabz_occ_mod.F90`





O. Jepsen and O. K. Andersen, Solid State Commun. 9, 1763 (1971)

$$V_T = \frac{V_{BZ}}{6N_k}$$

When we use linear interpolation, the next is satisfied.

If $\varepsilon_1 \le \varepsilon \le \varepsilon_2 \le \varepsilon_3 \le \varepsilon_4$,

$$\int_T \theta(\varepsilon - \varepsilon_k) = V_{\varepsilon_k \le \varepsilon} \approx V_T \frac{\varepsilon - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} \frac{\varepsilon - \varepsilon_1}{\varepsilon_3 - \varepsilon_1} \frac{\varepsilon - \varepsilon_1}{\varepsilon_4 - \varepsilon_1}$$

$$\int_T \delta(\varepsilon - \varepsilon_k) = \frac{\partial}{\partial \varepsilon} \int_T \theta(\varepsilon - \varepsilon_k)$$

If $\varepsilon_1 \le \varepsilon_2 \le \varepsilon \le \varepsilon_3 \le \varepsilon_4, \cdots$

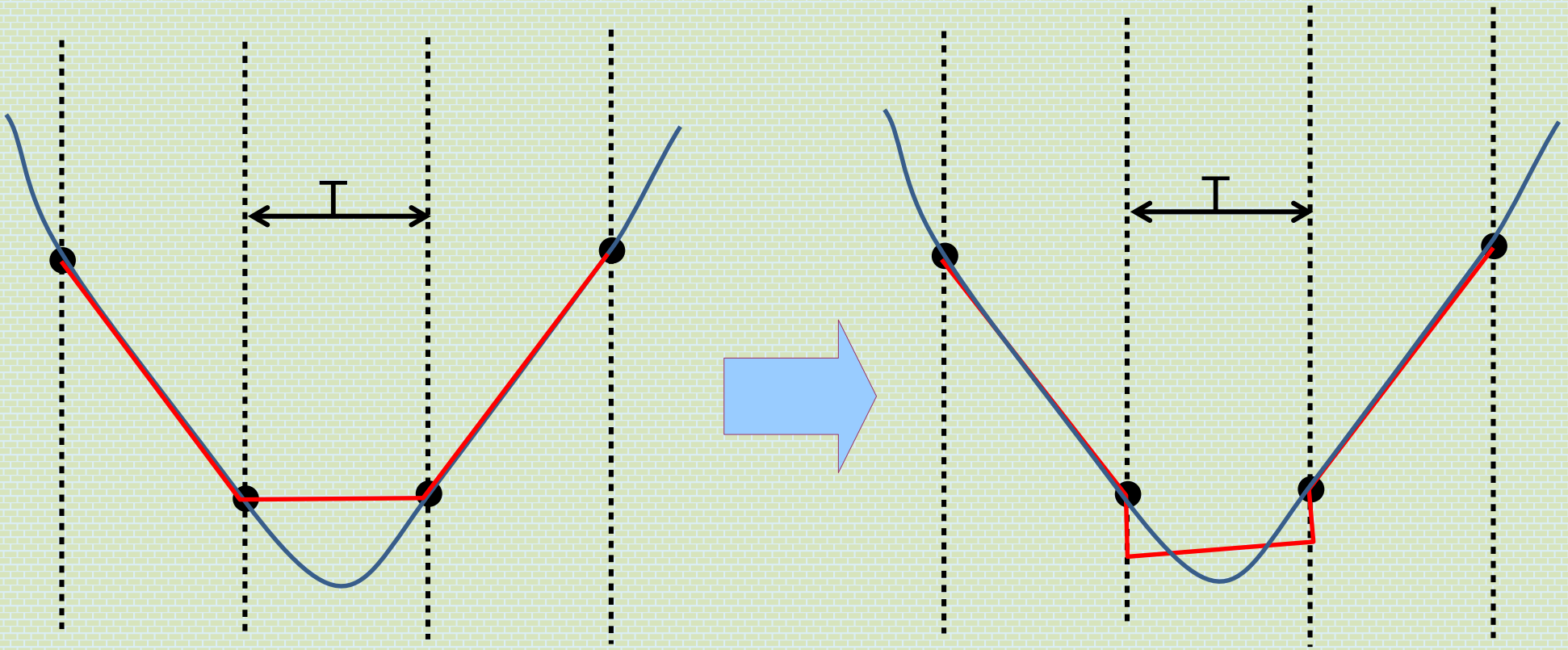
If $\varepsilon_1 \le \varepsilon_2 \le \varepsilon_3 \le \varepsilon \le \varepsilon_4, \cdots$

If $\varepsilon_1 \le \varepsilon_2 \le \varepsilon_3 \le \varepsilon_4 \le \varepsilon, \cdots$

These expressions are not applicable for higher order (2^{nd} , 3^{rd} ・・・) interpolation !

Systematic error in tetrahedron method

(Traditional) tetrahedron method linearly interpolate the function of k (such as wave function, KS energy, etc.).



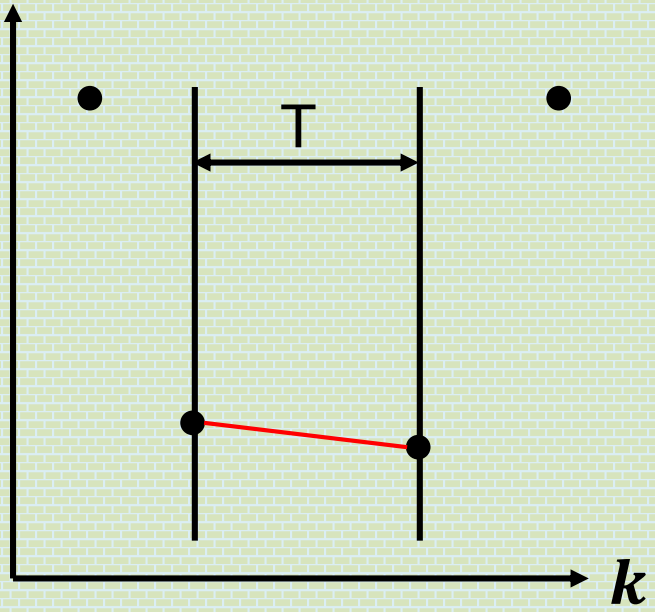
If the sign of curvature of these function is always negative, we overestimete.

Not Interpolating
But Fitting

Optimized tetrahedron method

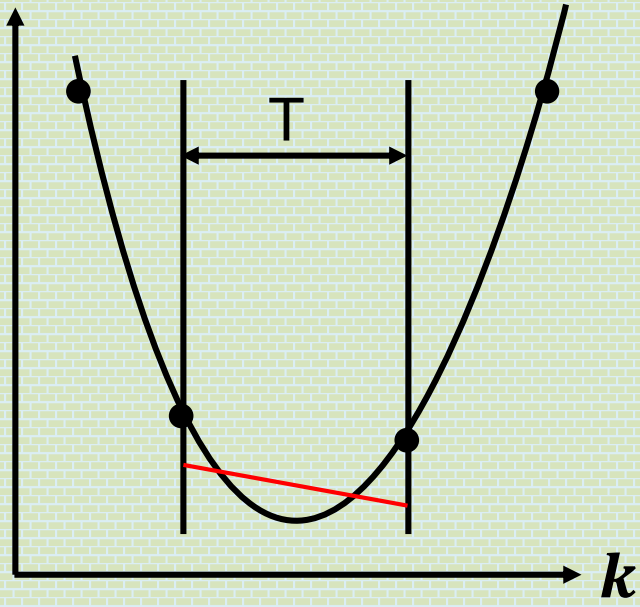
M. Kawamura *et al.*, Phys. Rev. B 89, 094515 (2014).

Conventional tetrahedron method



1. Linear interpolation of ε_k, etc.
2. Tetrahedron method with interpolated linear function

Optimized tetrahedron method



1. Higher order interpolation of ε_k , etc.
2. Fit this function into a linear function in the tetrahedron
3. Tetrahedron method with fitted linear function

Library of tetrahedron method

LibTetraBZ http://libtetrabz.osdn.jp/

Fortran/C/C++

$$\sum_{n}\int_{BZ}\frac{d^3k}{V_{BZ}}\delta(\varepsilon-\varepsilon_{n\boldsymbol{k}})\,X_{n\boldsymbol{k}}$$

$$\sum_{n}\int_{BZ}\frac{d^3k}{V_{BZ}}\theta(\varepsilon-\varepsilon_{n\boldsymbol{k}})X_{n\boldsymbol{k}}$$

$$\sum_{n,n'}\int_{BZ}\frac{d^3k}{V_{BZ}}\frac{\theta(\varepsilon'_{n'\boldsymbol{k}}-\varepsilon_F)\theta(\varepsilon_F-\varepsilon_{n\boldsymbol{k}})}{\varepsilon'_{n'\boldsymbol{k}}-\varepsilon_{n\boldsymbol{k}}}X_{nn'\boldsymbol{k}}$$

$$\sum_{n,n'}\int_{BZ}\frac{d^3k}{V_{BZ}}\theta(\varepsilon_F-\varepsilon'_{n'\boldsymbol{k}})\theta(\varepsilon_F-\varepsilon_{n\boldsymbol{k}})\delta(\varepsilon'_{n'\boldsymbol{k}}-\varepsilon_{n\boldsymbol{k}}+\omega)X_{nn'\boldsymbol{k}}(\omega)$$

$$\sum_{n,n'}\int_{BZ}\frac{d^3k}{V_{BZ}}\frac{\theta(\varepsilon_F-\varepsilon'_{n'\boldsymbol{k}})\theta(\varepsilon_F-\varepsilon_{n\boldsymbol{k}})}{\varepsilon'_{n'\boldsymbol{k}}-\varepsilon_{n\boldsymbol{k}}+i\omega}X_{nn'\boldsymbol{k}}(\omega)$$

MPI + OpenMP (Thread safe)

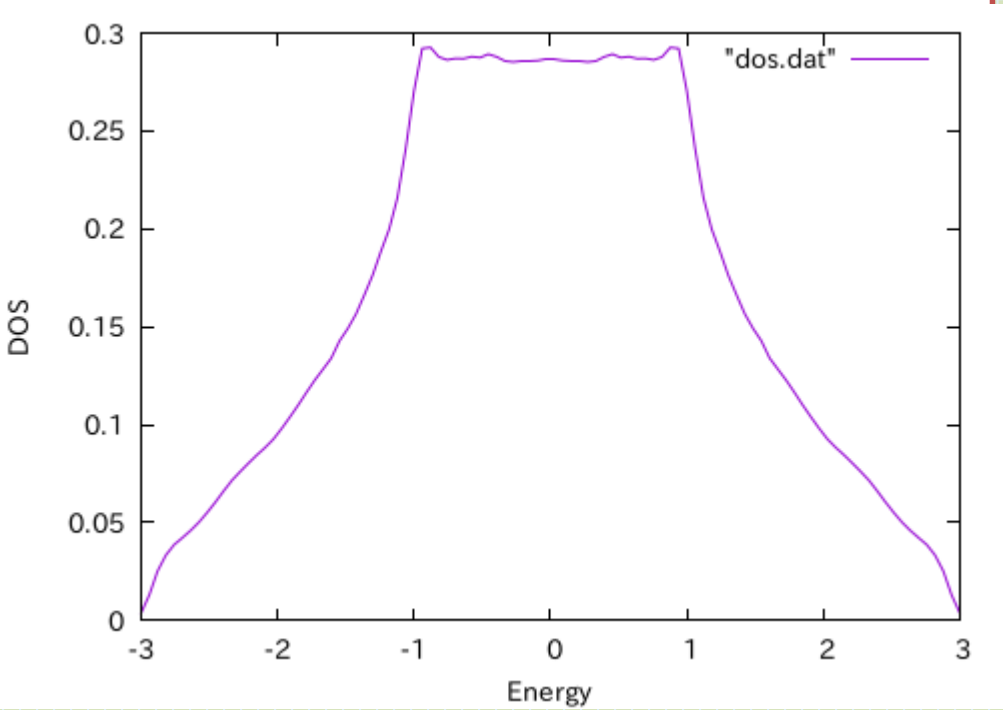
$$\sum_{n,n'}\int_{BZ}\frac{d^3k}{V_{BZ}}\delta(\varepsilon_F-\varepsilon_{n\boldsymbol{k}})\delta(\varepsilon_F-\varepsilon'_{n'\boldsymbol{k}})X_{nn'\boldsymbol{k}}$$

$$\sum_{n,n'}\int_{BZ}\frac{d^3k}{V_{BZ}}\theta(\varepsilon'_{n'\boldsymbol{k}}-\varepsilon_F)\theta(\varepsilon_F-\varepsilon_{n\boldsymbol{k}})X_{nn'\boldsymbol{k}}$$

LibTetraBZ

```
$ cd ~/
$ git clone git://git.osdn.net/gitroot/libtetrabz/libtetrabz.git
$ cd libtetrabz
$ touch Makefile.in aclocal.m4 configure
$ ./configure; make
$ cd example
$ ./dos.x
Which tetrahedron method ?(1 = Linear, 2 = Optimized): 2⏎
 k-point mesh ?: 10⏎
$ gnuplot
gnuplot> set xlabel "Energy"
gnuplot> set ylabel "DOS"
gnuplot> plot "dos.dat" w l
```

$$\varepsilon_k = -\cos k_x - \cos k_y - \cos k_z$$



Fermi energy with bisection method

`libtetrabz_fermieng@libtetrabz/src/libtetrabz_occ_mod.F90`

$$N = \sum_n \int_{BZ} \frac{d^3k}{V_{BZ}} \theta(\varepsilon_F - \varepsilon_{n\boldsymbol{k}})$$

$\varepsilon_{up} = \max\{\varepsilon_{nk}\}$ $\varepsilon_{low} = \min\{\varepsilon_{nk}\}$

do iteration

$\varepsilon_F = (\varepsilon_{up} + \varepsilon_{low})/2$

$$\widetilde{N} = \sum_n \int_{BZ} \frac{d^3k}{V_{BZ}} \theta(\varepsilon_F - \varepsilon_{n\boldsymbol{k}})$$

if $|\widetilde{N} < N|$ is small → Finish

else if $\widetilde{N} < N$

$\varepsilon_{low} = \varepsilon_F$

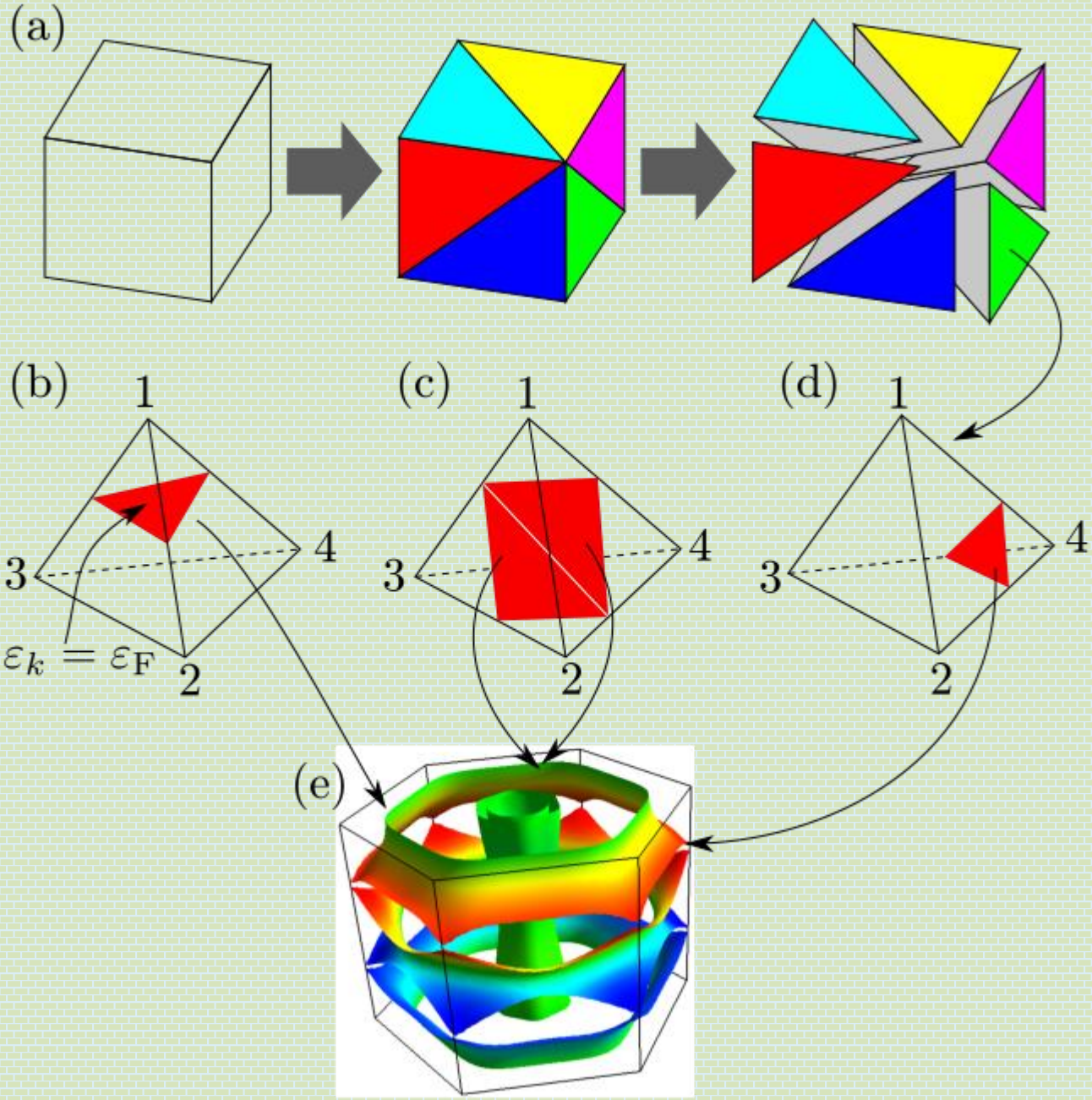
else if $\widetilde{N} > N$

$\varepsilon_{up} = \varepsilon_F$

end if

end do iteration

Iso surface with tetrahedron method



FermiSurfer

Input file format

http://fermisurfer.osdn.jp/en/_build/html/fermisf_input_en.html

Report problem 3

(1) Modify dos.F90 or dos_c.c to compute DOS with Gaussian broadening method.

$$\int_{BZ} \frac{d^3k}{V_{BZ}} \delta(\varepsilon - \varepsilon_{\boldsymbol{k}}) \approx \frac{1}{N_k} \sum_{k}^{N_k} \frac{1}{\sigma\sqrt{\pi}} e^{-\left(\frac{\varepsilon-\varepsilon_{\boldsymbol{k}}}{\sigma}\right)^2}$$

Plot DOS at each N_k and σ, then compare with tetrahedron methods (Linear and optimized)

Note:
Replace
```
call libtetrabz_fermieng(ltetra,bvec,nb,nge,eig,ngw,wght,ef,nelec)
```
to
```
ef = 0.0d0
```

(2) Output $\varepsilon_{\boldsymbol{k}}$ and $|\boldsymbol{\nabla}_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}}|$ in the FermiSurfer format (vf.frmsf).

Modified code should be submitted as a diff file generated by

```
$ cd ~/libtetrabz/
$ git add example
$ git commit
$ git show > 12212018.diff
```

Today's summary

- Total energy
  - Hartree, atomic, XC, kinetic, Ewald energy
  - Coulomb repulsion of periodically aligned ions is computed efficiently with Ewald's method.
- Brillouin zone integration
  - Tetrahedron method
  - Optimized tetrahedron method
  - Library
  - Fermi surface