Computational Materials Science (計算材料学特論)

http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE_programs.html?page=cms

COMPUTATIONAL MATERIALS SCIENCE 2026 Q2
2026年度Q2 計算材料学特論 (資料: 英語＋日本語版)

Lecture materials for numerical analyses (by Kamiya)
数値解析に関する講義資料・pythonプログラム (神谷担当分)

Update News:

- **June 19, 08:10, 2026:** Lecture materials for June 19 has been updated: course_materials.zip
- **June 18, 10:29, 2026:** Lecture materials for June 19 has been uploaded
- **June 16, 15:38, 2026:** Lecture videos have been moved to tutorial web
- **June 16, 15:38, 2026:** Final version: Lecture materials for June 16 has been updated: course_materi

FY2026

#03 June 19, 2026: Differential equation (微分方程式), Interpolation (補間 method (線形最小二乗法)

Course materials (Lecture slides and python programs):

- course_materials.zip

5-8min audio guide:

- 日本語: 0:00 / 5:16 (VOICEVOX 四国めたん&ずんだもん)
- English: 0:00 / 4:27

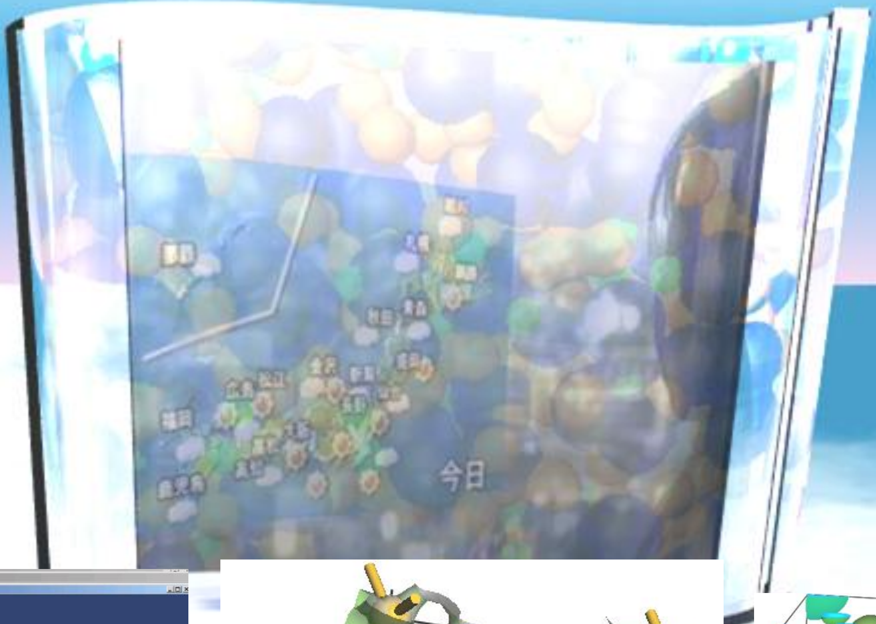
#02 June 16, 2026: Numerical differentiation (数値微分), Numerical integration(数値積分), Differenti 式)

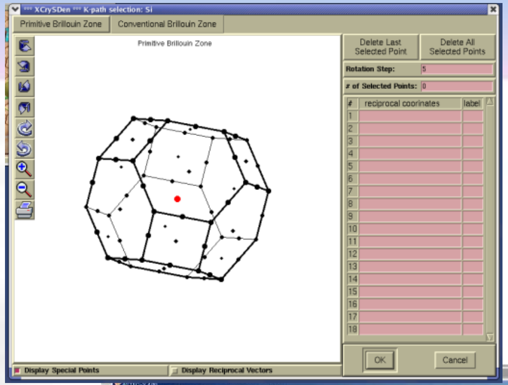
We would wait for five minuities (i.e., till 8:55).
In meantime
- **download the latest lecture materials (updated this morning)**
- **hear the short audio guide. English and Japanese versions available**

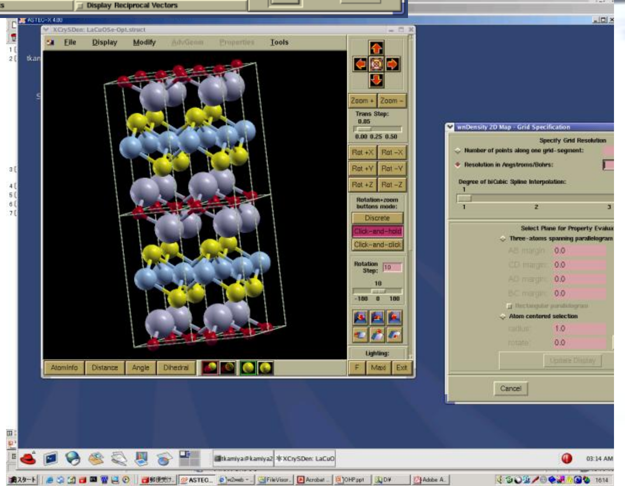
MAT.C505

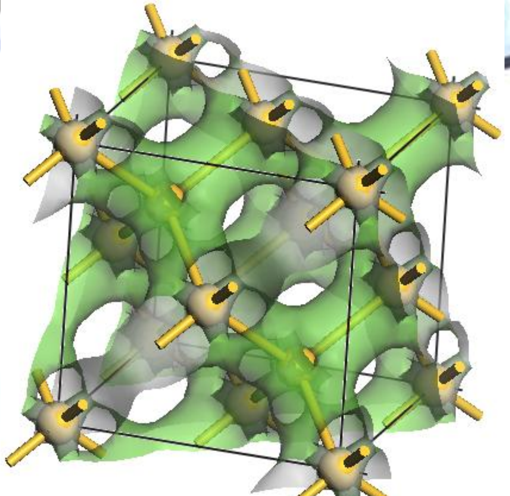
Computational Materials Science
計算材料学特論

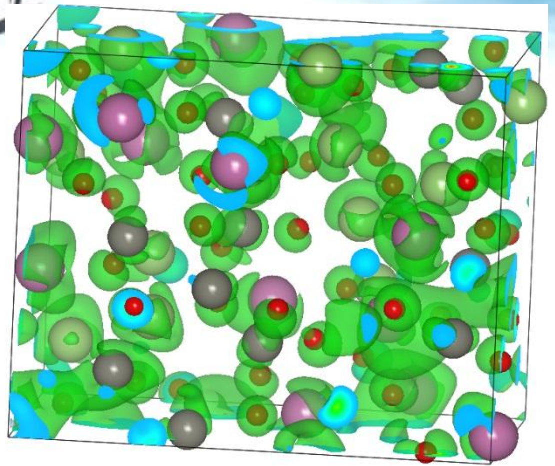
Toshio Kamiya
神谷利夫











Class Schedule

Lecture materials (Kamiya's part): **http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/?page=cms**

授業 6月10日(水)～7月28日(火), 7月30日(木) 月曜の授業 7月23日(木) 期末試験･補講 7月29日(水), 7月31日(金)～8月6日(木)

#01 June 12 (Fri) Kamiya (Fundamentals of computer, Sources of error (コンピュータの基礎、誤差), Numerical differentiation (数値微分))

#02 June 16 (Tue) Kamiya (Numerical differentiation (数値微分), Numerical integration (数値積分), Differential equation (微分方程式))

#03 June 19 (Fri) Kamiya (Differential equation (微分方程式), Molecular dynamics (分子動力学法), Interpolation (補間), Smoothing (平滑化), Linear least-squares method (線形最小二乗法))

#04 June 23 (Tue) Kamiya (Linear least-squares method (線形最小二乗法), Optimization (最適化), Numerical solutions of equations (方程式の数値解法), Nonlinear optimization (非線形最適化))

#05 June 26 (Fri) Kamiya (Nonlinear optimization (非線形最適化), Fourier transformation (フーリエ変換)

#06 June 30 (Tue) Kamiya, Matrix (行列)

#07 July 3 (Fri) Kamiya, Review (復習)

#08 July 7 (Tue) Sasagawa (Review of quantum theory 1: 量子論おさらい1)

#09 July 10 (Fri) Sasagawa (Review of quantum theory 2: 量子論おさらい2)

#10 July 14 (Tue) Sasagawa (First principles calculations: basics 1 第一原理計算:基礎1)

#11 July 17 (Fri) Sasagawa (First principles calculations: basics 2 第一原理計算:基礎2)

#12 July 2 (Fri) Sasagawa (First principles calc.: applications 1 第一原理計算:応用1)

#13 July 24 (Fri) Sasagawa (First principles calc.: applications 2 第一原理計算:応用2)

#14 July 28 (Fri) Sasagawa (Classical and Quantum Computers 古典および量子コンピュータ)

Explanation of the answers

課題解答の解説

PROBLEM, June 16

- **Answer in English or Japanese**
- **Submit electronic file(s) via LMS until June 17**

(If LMS doesn't work, send the files to kamiya.t.aa@m.titech.ac.jp.
In this case, file name must include your STUDENT ID and FULL NAME)

PROBLEM:

(i) Calculate d$E(k)$/dk, d$^2E(k)$/dk^2, and effective mass m_e^*/m_0 from $E(k)$ in band.xlsx, and plot m_e^*/m_0 vs k.
Assume the lattice parameter is a = 4.0 Å.
(ii) Compare the results obtained by different h.

Optional: Any questions and impressions of the lecture style are welcome

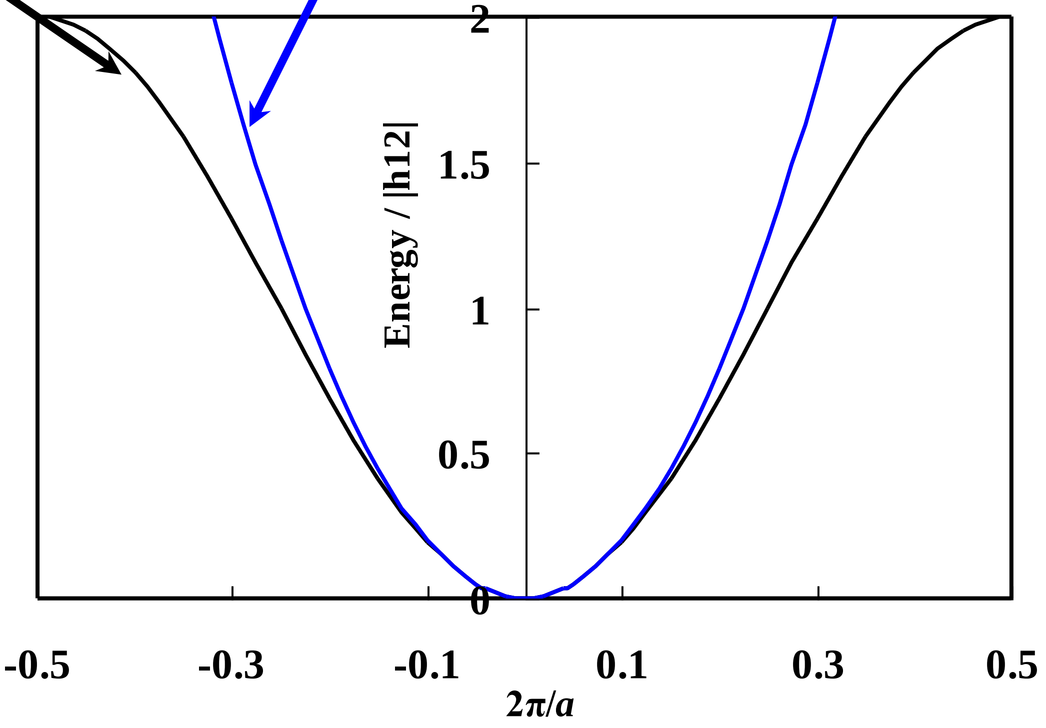
Effective mass

LCAO band

$$E(k) = \varepsilon_1 - 2|h_{12}|\cos(ka) \sim \varepsilon_1 - 2|h_{12}| + |h_{12}|a^2k^2 + O((ka)^4)$$

Free electron model

$$E(k) = E_0 + \frac{|\mathbf{P}|^2}{2m} = E_0 + \frac{\hbar^2}{2m}|\mathbf{k}|^2$$



$$\boxed{\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E_n(\mathbf{k})}{\partial k^2}}$$

Calculation of effective mass from $E(k)$

k represents fractional coordinate in reciprocal unit cell: generally expressed in the range **[-½ ½]**

Unit conversion $\boldsymbol{k_{real} = (2\pi/a)k}$, **$E(k)$ is in eV**

$$m^* = \hbar^2 \left(\frac{\partial^2 E_n(\mathbf{k})}{\partial {k_{real}}^2} \right)^{-1} = \hbar^2 \left(\frac{2\pi}{a} \right)^2 \left(\frac{\partial^2 E_n(\mathbf{k})}{\partial k^2} \boldsymbol{e} \right)^{-1}$$

Very often effective mass is given by a ratio to the electron rest mass m_e^0.

$$m^*/{m_e}^0 = \hbar^2 \left(\frac{\partial^2 E_n(\mathbf{k})}{\partial {k_{real}}^2} \right)^{-1} /{m_e}^0 = \hbar^2 \left(\frac{2\pi}{a} \right)^2 \left(\frac{\boldsymbol{\partial^2 E_n(k)}}{\boldsymbol{\partial k^2}} \boldsymbol{e} \right)^{-1} /{m_e}^0$$

Numerical differentiation: 3-point formula

$$\frac{df(x_i)}{dx} \sim = \frac{f(x_i+h) - f(x_i-h)}{2\Delta t}$$

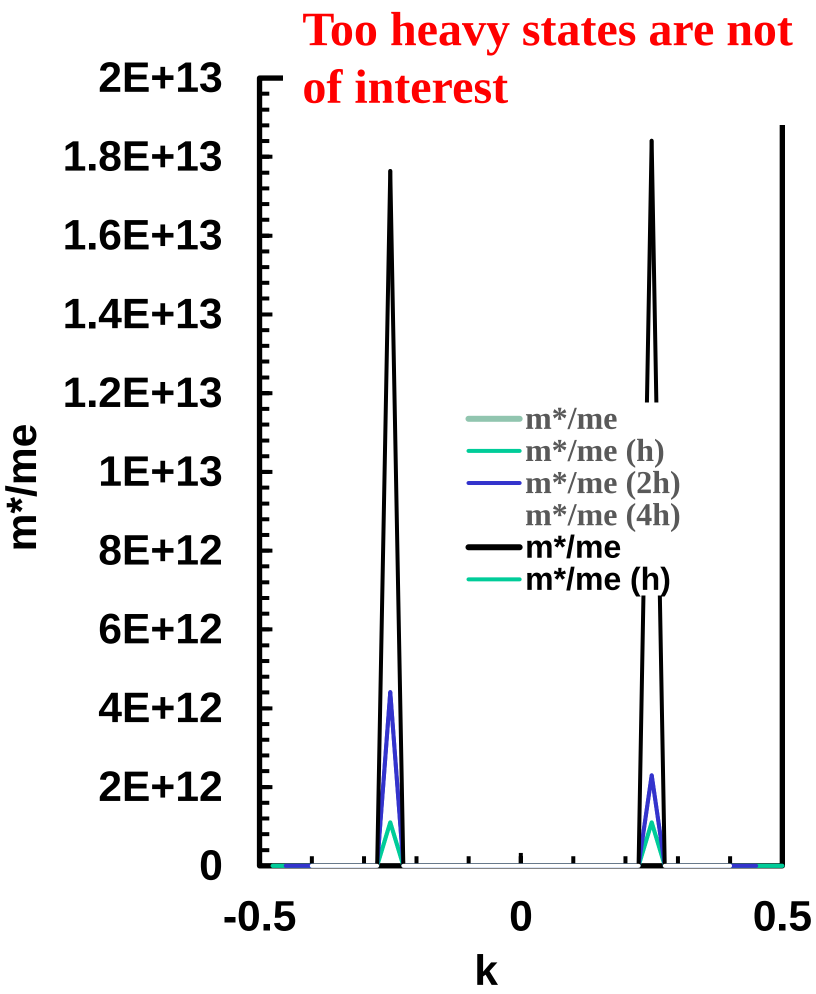
$$\boldsymbol{\frac{d^2 f(x_i)}{dx^2} \sim = \frac{f(x_i+h) - 2f(x_i) + f(x_i-h)}{h^2}}$$

Check convergence by decreasing *h*

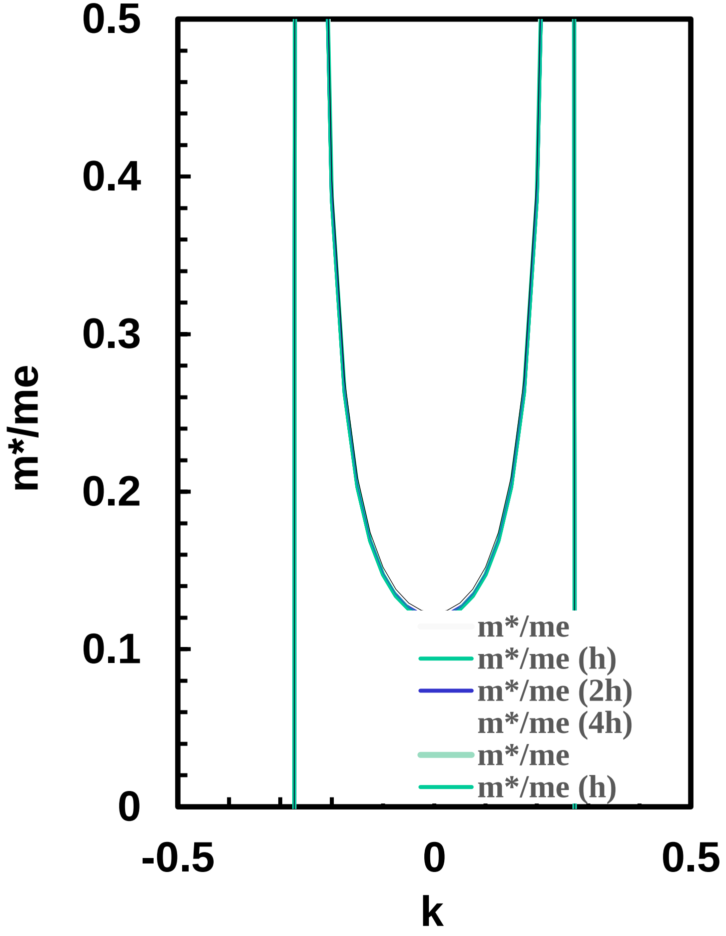
Answer: How to present?

band-answer.xlsx

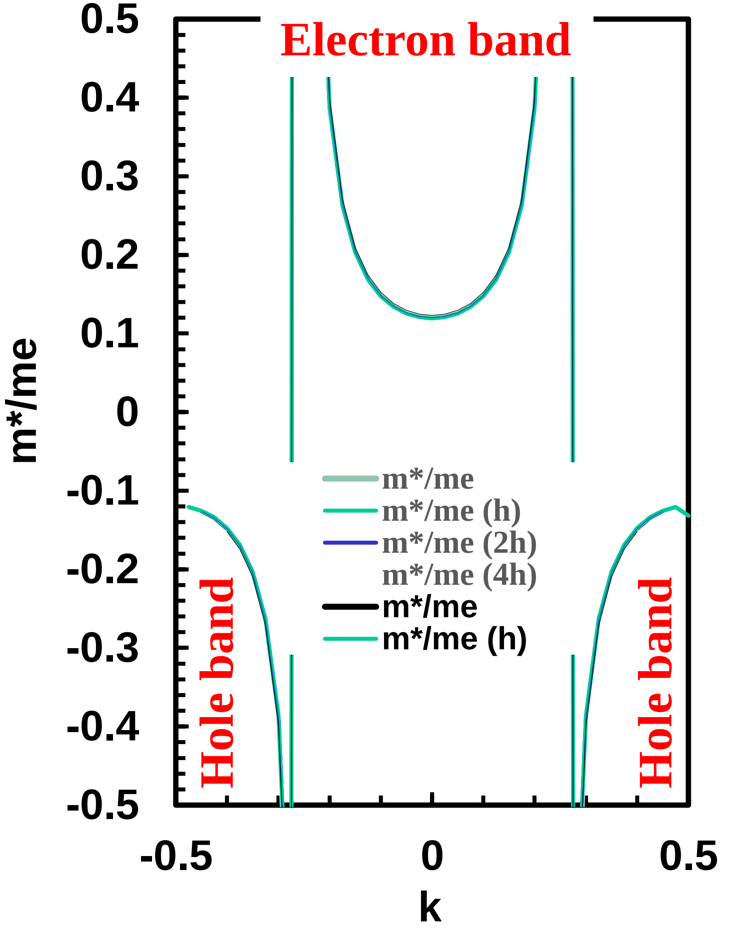
Full range



Electron only ($m^* > 0$)



Electron and holes



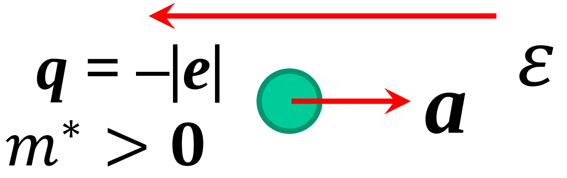
Negative effective mass

Semiclassical equation of motion for an electron in a band $\boldsymbol{E(k)}$:

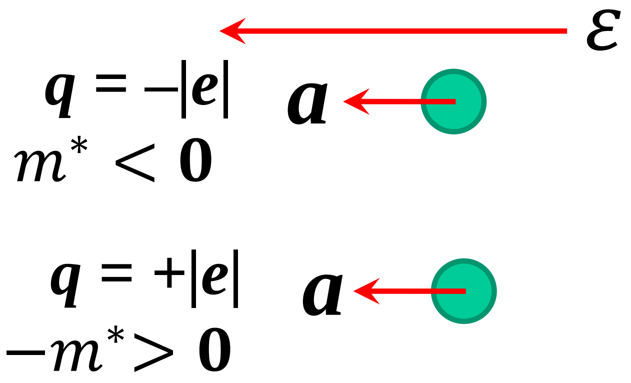
Acceleration theorem: $\boldsymbol{F} = \hbar \frac{d\boldsymbol{k}}{dt} = m^* \frac{d^2\boldsymbol{r}}{dt^2}$

$$\boldsymbol{v} = \frac{1}{\hbar}\frac{dE(\boldsymbol{k})}{d\boldsymbol{k}} \qquad \boldsymbol{a} = \frac{\mathrm{d}\boldsymbol{v}}{dt} = \frac{1}{\hbar}\frac{d^2E(\boldsymbol{k})}{d\boldsymbol{k}^2}\frac{d\boldsymbol{k}}{dt} = \frac{\boldsymbol{F}}{\hbar^2}\frac{d^2E(\boldsymbol{k})}{d\boldsymbol{k}^2} = \frac{\boldsymbol{F}}{m^*} \qquad \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E(\boldsymbol{k})}{d\boldsymbol{k}^2}$$

For electron under an electric field ε: $\boldsymbol{F} = -|e|\boldsymbol{\varepsilon}$



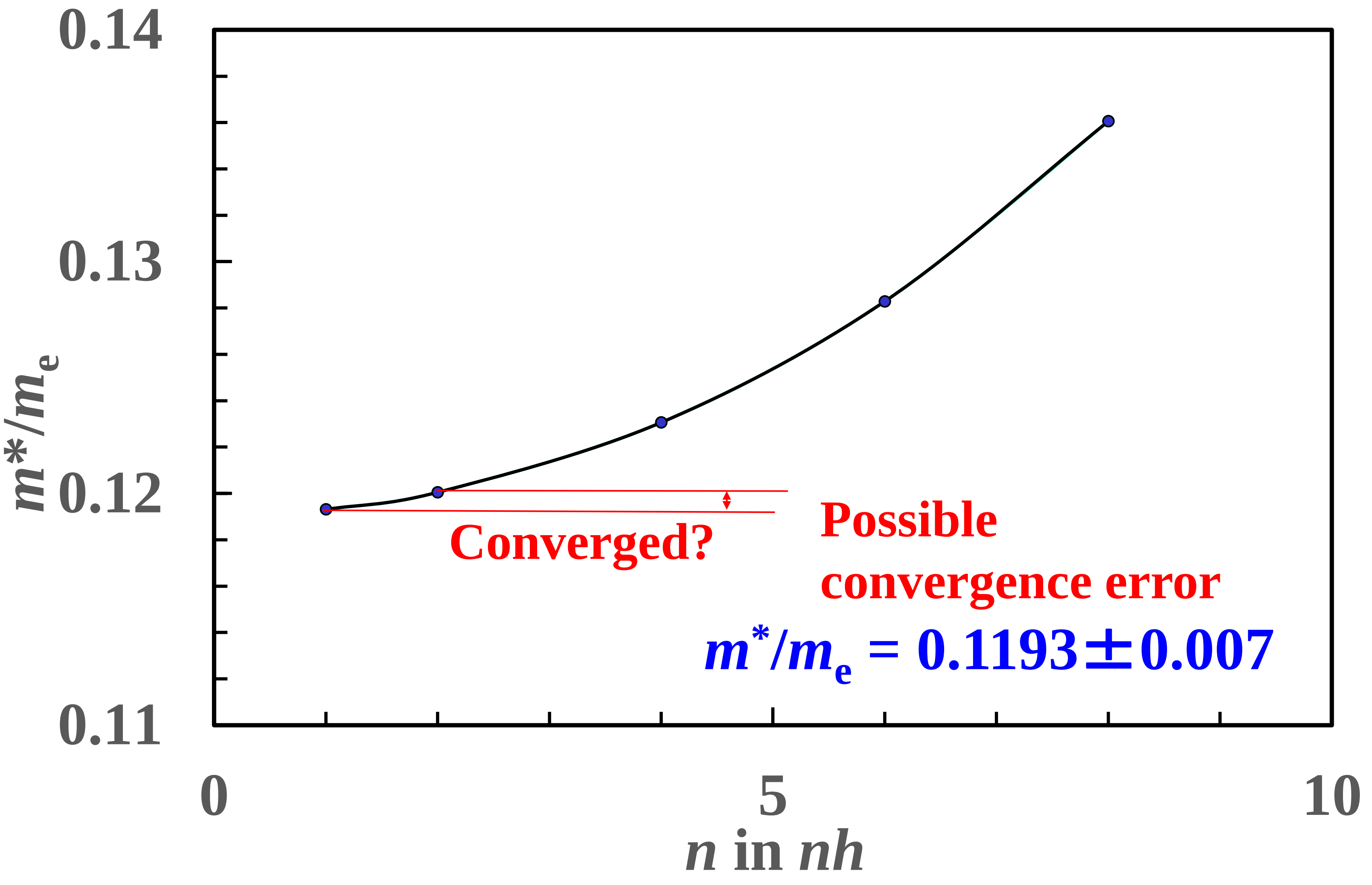
Negative effective mass: $-|e|\boldsymbol{\varepsilon} = -|m^*|\frac{d^2\boldsymbol{r}}{dt^2}$ => $+|e|\boldsymbol{\varepsilon} = |m^*|\frac{d^2\boldsymbol{r}}{dt^2}$



Regarded as a hole with positive charge |*e*|

Accuracy and convergence check

band-answer.xlsx

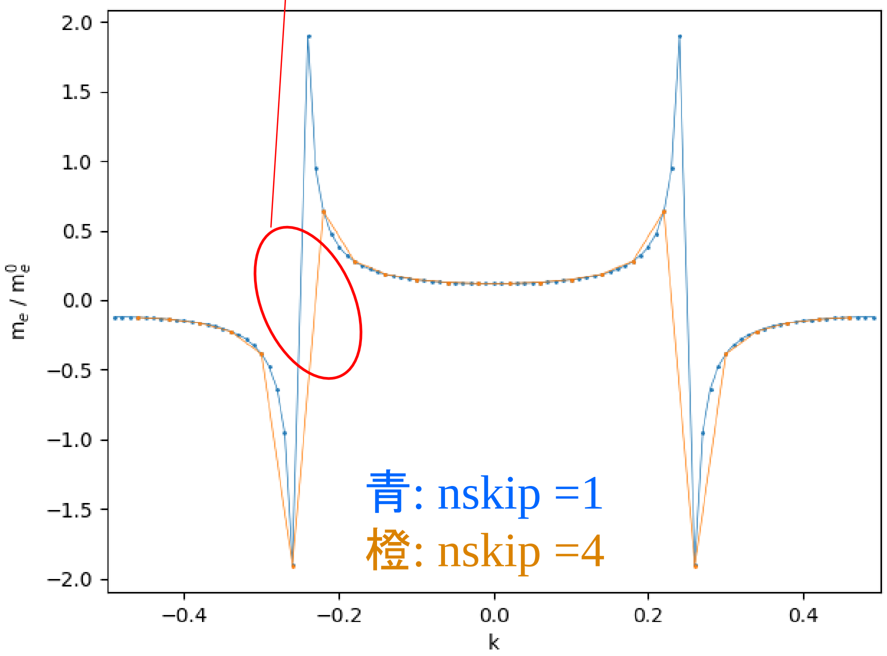


h	m*/me
1	0.119310839
2	0.120049846
4	0.123061372
6	0.128284879
8	0.136053307

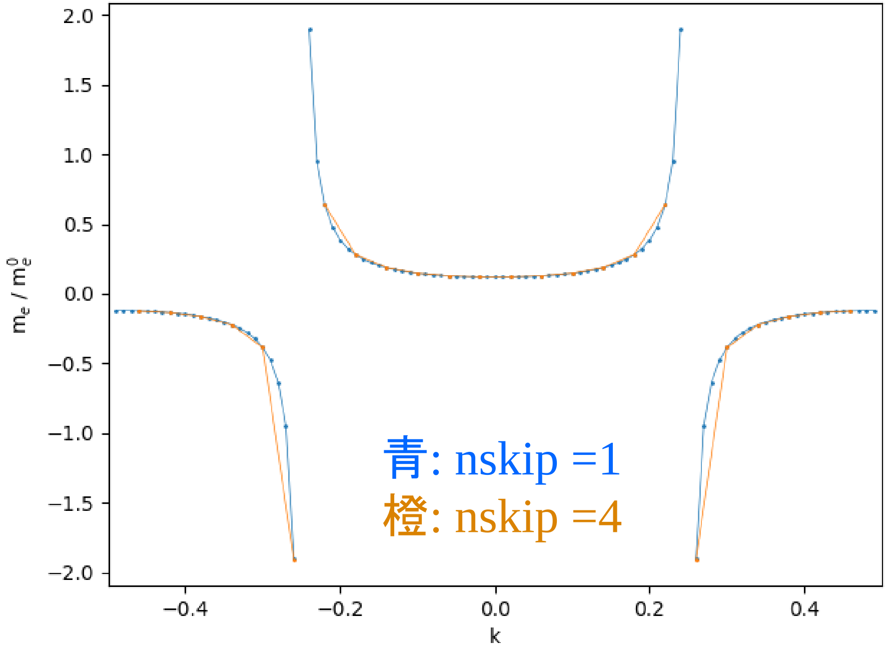
Python program (抜粋)

python EffectiveMass.py

These lines should not be drawn
描いてはいけない線



Data points can be disconnected by inserting None values
データに None (未定義値) を挿入することで描いてはいけない線を消した



Python program (抜粋)

EffectiveMass.py

```
#共通の定数は先に計算
  km = hbar * hbar * (pi2 / a)**2.0
#微分の精度を比較するため、h = nskip*dk にする
   nskip = 1
   xk  = []
   ymc = []
#符号の変化を検出するため、符号変数を用意
signprev = None
for i in range(nskip, nk - nskip, nskip):
#2階微分を計算
      d2Edk2c = (E[i+nskip] + E[i-nskip] - 2 * E[i]) * e / pow(nskip * dk, 2.0)
#2回微分はゼロになることがあるので、まずは1/m*を計算
      minv = d2Edk2c / km
      print(i, E[i-1], E[i], E[i+1], minv)
#1/m*が1/meより非常に小さければ、m*は計算しない
      if abs(minv) <= 1.0e20:  # << 1.0/me ~ 1e30
#符号が反転する場所でグラフの線を切断するときは
#Noneデータを追加する。
         if cutline:
            xk.append(k[i])
            ymc.append(None)
#反転した符号を記録
            signprev = -signprev
            continue
      else:
         m = km / d2Edk2c
#符号が反転する場所でグラフの線を切断するときは
#Noneデータを追加する。
         if signprev is None:
#signprevが 初期値 None である場合は 符号の最初の値を代入
            signprev = m
         elif signprev * m < 0.0:
            if cutline:
               xk.append(k[i])
               ymc.append(None)
#反転した符号を記録
            signprev = m

         xk.append(k[i])
         ymc.append(m / me)

   plt.plot(xk,  ymc,  linewidth = 0.5, marker = 'o', markersize = 1.0, label = 'nskip = 1')
   plt.xlabel(klabel)
   plt.ylabel("m$_e$ / m$_e^0$")
   plt.xlim([-0.5, 0.5])
#   plt.ylim([-0.5, 0.5])
   plt.tight_layout()

   plt.pause(0.1)
   print("Press ENTER to exit>>", end = '')
   input()


if __name__ == "__main__":
   main()
```

PROBLEM, June 19

- **Answer in English or Japanese**
- **Submit electronic file(s) via LMS until the midnight of June 21**

  (If LMS doesn't work, send the files to kamiya.t.aa@m.titech.ac.jp.
  In this case, file name must include your STUDENT ID and FULL NAME)
- Common formats (.pdf, .txt., .docx, .xlsx, .pptx) are acceptable,
  but NO APPLE-ONLY files

PROBLEM:

(i) By filling the *dx*/*dt* and the *x*(*t*) columns in diffeq.xlsx,
solve $dx(t) / dt = -x(t)\sin(\pi t)$ using the Euler method.

Conditions:

t starts from 0 and ends at 3.0 with the time step of 0.1.

$x(0) = 1.0$

Optional: Any questions and impressions of the lecture style are welcome