jupyter

December 1, 2024

[1]:
```
import scipy.constants as c
from IPython.display import display as print
from sympy import *
init_printing(use_latex="mathjax")
```

[2]:
```
# Nr 1 (a)
sigma, epsilon, r, r_0, beta, k_B, T = symbols("sigma epsilon r r_0 beta k_B␣
↪T",positive=True)
V = 4*epsilon*((sigma/r)**12 - (sigma/r)**6)
D_2 = V.diff(r,2).subs(r,2**(Rational(1,6))*sigma)
D_3 = V.diff(r,3).subs(r,2**(Rational(1,6))*sigma)
print(D_2,D_3)
```

$$\frac{36 \cdot 2^{\frac{2}{3}} \epsilon}{\sigma^2}$$

$$-\frac{756\sqrt{2}\epsilon}{\sigma^3}$$

[3]:
```
# (b)
weight = exp(-beta * D_2/2 * (r-r_0)**2) * (1 - beta * D_3/6 * (r-r_0)**3)
Z = Integral(weight, (r,-oo,oo)).doit()
rZ = simplify(Integral(r*weight, (r,-oo,oo)).doit().subs(r_0,␣
↪2**Rational(1,6)*sigma))
x_ev = simplify(rZ/Z)
print(Z,rZ,x_ev)
```

$$\frac{\sqrt[6]{2}\sqrt{\pi}\sigma}{6\sqrt{\beta}\sqrt{\epsilon}}$$

$$\frac{\sqrt[3]{2}\sqrt{\pi}\sigma^2 \cdot (48\beta\epsilon + 7)}{288\beta^{\frac{3}{2}}\epsilon^{\frac{3}{2}}}$$

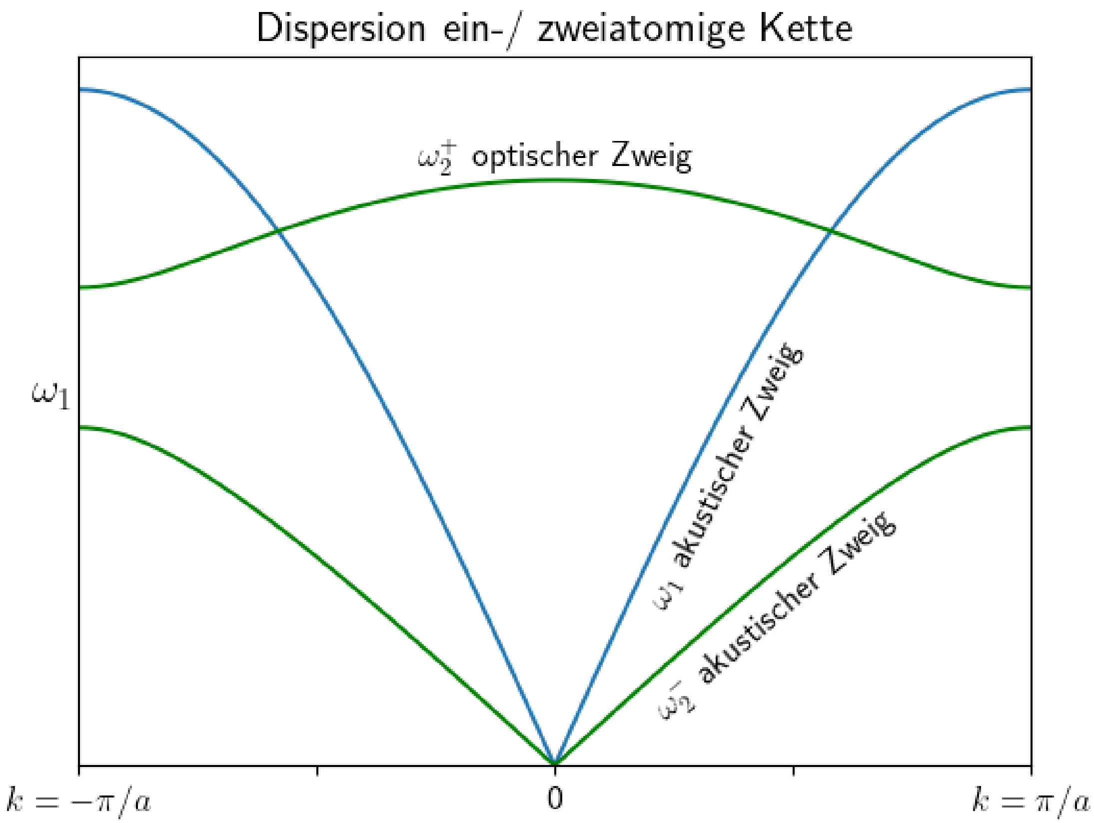
$$\frac{\sqrt[6]{2}\sigma\,(48\beta\epsilon + 7)}{48\beta\epsilon}$$

[4]:
```
# (c)
alpha = 7*c.Boltzmann / (48 * 10e-3 * c.e)
alpha
```

[4]:

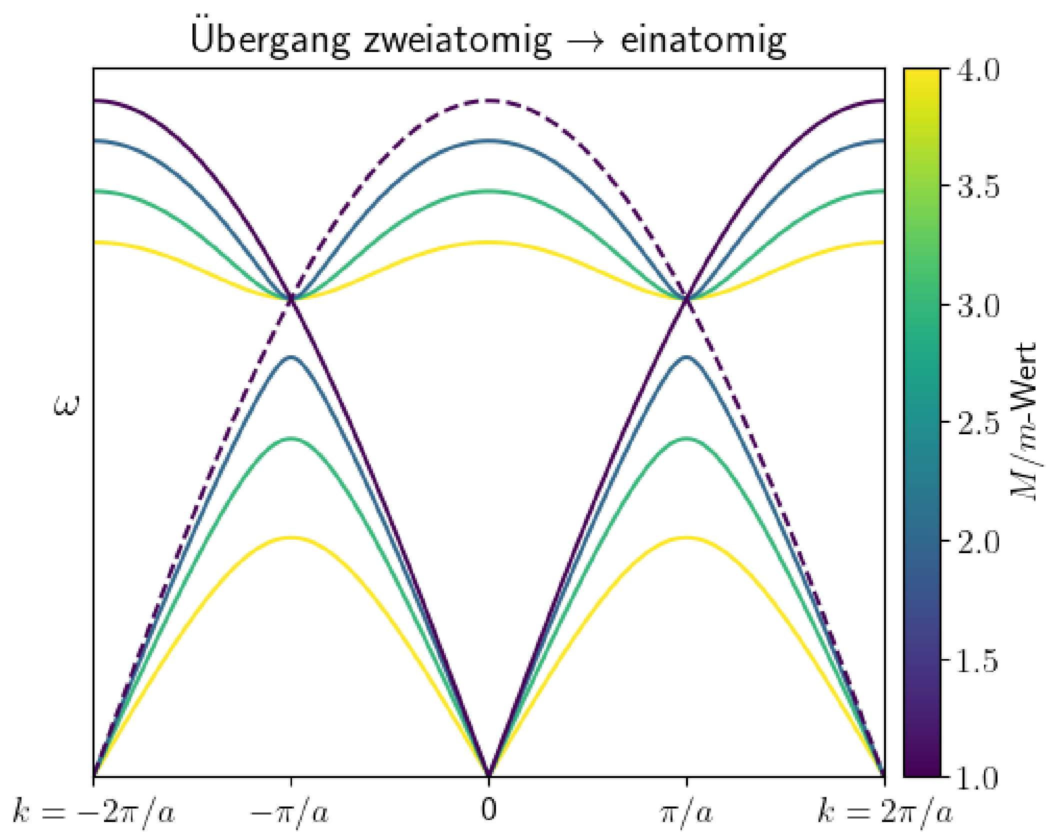
0.001256694434406284

[5]:
```python
# Nr 2 (a)
import numpy as np
import matplotlib.pyplot as plt
plt.rcParams.update({
                     "text.usetex": True, "font.size": 13
                     })

k = np.linspace(-np.pi,np.pi,1000)
omega1 = np.sqrt(4 *np.sin(k/2)**2)
omega2optical = np.sqrt(3/2 + np.sqrt((3/2)**2 - 2*np.sin(k/2)**2))
omega2acoustic = np.sqrt(3/2 - np.sqrt((3/2)**2 - 2*np.sin(k/2)**2))

fig,ax = plt.subplots()
ax.plot(k, omega1)
ax.plot(k, omega2acoustic, c="g")
ax.plot(k, omega2optical,c="g")
plt.text(0,1.78, r"$\omega_2^+$ optischer Zweig",ha="center")
plt.text(1.44,0.14, r"$\omega_2^-$ akustischer Zweig",ha="center",rotation=41)
plt.text(1.12,0.47, r"$\omega_1$ akustischer Zweig",ha="center",rotation=63)
ax.set(ylim=(0,2.1),xlim=(-np.pi,np.pi),xticks=[-np.pi,-np.pi/2,0,np.pi/2,np.
 ↪pi],xticklabels=[r"$k=-\pi/a$","","0","",r"$k=\pi/
 ↪a$"],yticks=[],title="Dispersion ein-/ zweiatomige Kette")
ax.set_ylabel(r"$\omega_1$",rotation=0,labelpad=10,size=16)
fig.savefig("dispersion.pdf")
```



[6]:
```
from matplotlib.cm import ScalarMappable
from matplotlib.colors import LinearSegmentedColormap

M = [4, 2, 1.3, 1]
N = len(M)
cmap = plt.cm.viridis
c = cmap(np.linspace(1, 0, N))
k = np.linspace(-2*np.pi, 2*np.pi, 1000)

omega1 = lambda k,M: np.sqrt(4 *np.sin(k/2)**2)
omega2optical = lambda k,M: np.sqrt((1/M + 1) + np.sqrt(((1/M + 1))**2 - 4/M *␣
↪np.sin(k/2)**2))
omega2acoustic = lambda k,M: np.sqrt((1/M + 1) - np.sqrt(((1/M + 1))**2 - 4/M *␣
↪np.sin(k/2)**2))

fig, ax = plt.subplots()
for i in range(N-1):
    ax.plot(k, omega2acoustic(k,M[i]), c=c[i])
    ax.plot(k, omega2optical(k,M[i]), c=c[i])
ax.plot(k, omega1(k/2, M[-1]), c=c[-1])
```

```
ax.plot(k, omega1(k/2+np.pi, M[-1]), c=c[-1],linestyle="--")
ax.set(
    ylim=(0, 2.1),
    xlim=(- 2*np.pi, 2*np.pi),
    xticks=[-2*np.pi, -2*np.pi/2, 0, 2*np.pi/2, 2*np.pi],
    xticklabels=[r"$k=-2\pi/a$", r"$-\pi/a$", "0", r"$\pi/a$", r"$k=2\pi/a$"],
    yticks=[],
    title="Übergang zweiatomig $\\to$ einatomig"
)
ax.set_ylabel(r"$\omega$", rotation=0, labelpad=10, size=16)

sm = ScalarMappable(cmap=cmap, norm=plt.Normalize(vmin=min(M), vmax=max(M)))
sm.set_array([])
cbar = fig.colorbar(sm, ax=ax, pad=0.02)
cbar.set_label("$M/m$-Wert")

fig.savefig("transition.pdf")
plt.show()
```



[7]:
```python
# Nr.3 (a)
D_1,D_2,m,M,a,k = symbols("D_1 D_2 m M a k", positive=True)
k = symbols("k")
omega = sqrt((D_1+D_2)/m - 1/m * sqrt(D_1**S(2) + D_2**S(2) +
  2*D_1*D_2*cos(k*a)))
f = sqrt(D_1**2 + D_2**2 + 2*D_1*D_2*cos(a*k))
series(f,k,0,3)
```

[7]:

$$\sqrt{D_1^2 + 2D_1D_2 + D_2^2} - \frac{D_1D_2a^2k^2}{2\sqrt{D_1^2 + 2D_1D_2 + D_2^2}} + O\left(k^3\right)$$

[8]:
```python
# Nr.4 (a)
import scipy.constants as c
a = 3.61e-10
v = 4300
omega_max = 2*v/a # THz
print(f"{omega_max*1e-12 = :.3} Hz")

# (b)
E_max = c.hbar*omega_max/c.e# meV
print(f"{E_max*1e3 = :.3} eV")
```

```
'omega_max*1e-12 = 23.8 Hz'
```

```
'E_max*1e3 = 15.7 eV'
```

[9]:
```python
# Nr.5
lamb = 694e-9
n = 1.54
v = 6000

# (a)
k = n*2*np.pi/lamb
Delta_k = 2*n*2*np.pi/lamb
Delta_p = c.hbar * Delta_k
print(k,Delta_k,Delta_p)

# (b)
omega = v * Delta_k
print(omega)

# (c)
Delta_E_rel = omega / (2*np.pi*c.c/lamb)
print(Delta_E_rel)
```

13942514.9467674

27885029.8935348

$2.94067666599424 \cdot 10^{-27}$

167310179361.209

$6.16426447926185 \cdot 10^{-5}$