Set #6

17. *Radial Current Density.*

Problem 4.6. At instant $t = 0$ the electron behavior is described by the following wavefunction:

$$\Psi(r,0) = Ae^{-r^2/\alpha^2+ikr}\,. \tag{4.32}$$

Find the normalization constant, A, the most probable value r_{pr}, and the radial part of the probability current, j.

18.

The reflection and transmission coefficient of a dielectric slab of thickness "d" are:

$$r = \frac{(n^2-1)\,(e^{2ikdn}-1)}{(n+1)^2-(n-1)^2e^{2ikdn}} \qquad t = \frac{4n\,e^{ikdn}}{(n+1)^2-(n-1)^2e^{2ikdn}}$$

A non absorbing photonic crystal with n=2 (real) is made up of a periodic distribution of dielectric slabs whose thickness is $d = 0.1\,a$ alternated by vacuum regions. The structure periodicity is a.

a. Find the equation that describes the photonic band gap in terms of ωa/c.
b. Plot (Python, Mathematica, Matlab etc.) such an equation as a function of ωa/c.
c. Would an incident light beam with frequency such that ωa/c=3 e ωa/c=4 propagate or not?

19. Electrons may tunnel from a metal through the application of a suitable (constant) external electric field ε. After the application of the electric field ε the potential at the metal surface taken at x=a reads as (see class notes)

$$V(x) = E_F + \Phi - e\mathscr{E}(x-a)$$

Assuming that the tunneling electrons originates from a single-electronic state, estimate the field strength ε (volt/cm) needed to draw (*tunneling*) current densities of the order of mA/cm² from a potassium sample surface.

✧ Radial Current Density

Problem 4.6. At instant $t = 0$ the electron behavior is described by the following wavefunction:

$$\Psi(r, 0) = Ae^{-r^2/\alpha^2 + ikr} . \tag{4.32}$$

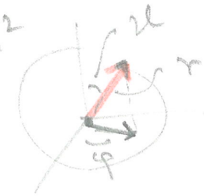
Find the normalization constant, A, the most probable value r_{pr}, and the radial part of the probability current, j.

$\psi(\bar{r},t) \to \psi(\bar{r},0) \equiv A e^{-r^2/\alpha^2} e^{ikr}$ 3D problem (general)

r = radial coordinate

a) $\int d\bar{r}\, |\psi(\bar{r},t)|^2 = \int d\bar{r}\, |\psi(\bar{r},0)|^2$ use polar coordinate (r,θ,φ)

$$= \int_0^{\infty} r^2 dr \int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\varphi\, |\psi(r,0)|^2$$



$$= 4\pi \int_0^{\infty} dr\, r^2 |\psi(r,0)|^2$$

or: $= 1$

$$4\pi |A|^2 \int_0^{\infty} r^2 dr\, e^{-2r^2/\alpha^2} = 4\pi |A|^2 \frac{\alpha^3}{8}\sqrt{\frac{\pi}{2}} = 1 \Rightarrow |A|^2 = \left(\frac{2}{\pi\alpha^2}\right)^{3/2}$$

b) most probable position occurs when prob. $|\psi(\bar{r},0)|^2 d\bar{r}$ is max:

$$\frac{d}{dr}\left(4\pi r^2 |\psi(r,0)|^2\right) = 4\pi |A|^2 \frac{d}{dr}\left(r^2 e^{-2r^2/\alpha^2}\right) = 0 \Rightarrow r_0 = \alpha/\sqrt{2}$$

c) Prob. current. In general $\bar{J}(\bar{r},t) = e\bar{v}\, |\psi(\bar{r},t)|^2$

At $t=0$ $\bar{J}(\bar{r},0) = e\bar{v}\, |\psi(\bar{r},0)|^2$; prob. density depends only on the radial coordinate so $\bar{J}(\bar{r},0) = e\, v_{rad} |\psi(r,0)|^2 \hat{\rho} = e\, v_{rad} \left(\frac{2}{\pi\alpha^2}\right)^{3/2} e^{-2r^2/\alpha^2} \hat{\rho}$

$$v_{rad} = \frac{p_{rad}}{m} \to \frac{1}{m} \mathrm{Re}\left[\int \psi^*(\bar{r},t) \underbrace{\left[-i\hbar \frac{\partial}{\partial r}\right]}_{\text{radial component of the } e^- \text{ momentum}} \psi(\bar{r},t)\right] = \dots = \mathrm{Re}\left[-\frac{i\hbar}{m} \int d\bar{r}\, \psi^*(r,0) \frac{\partial}{\partial r} \psi(r,0)\right]$$

$\boxed{\text{Review This} < >}$

Vol element: $r^2 dr \sin\theta\, d\theta\, d\varphi$

Now:

$$[..] = -\frac{i\hbar |A|^2}{m} 4\pi \int_0^{\infty} r^2 dr\, e^{-r^2/\alpha^2 - ikr} \left[e^{-r^2/\alpha^2}(+ik) + e^{-r^2/\alpha^2}\left(-\frac{2r}{\alpha^2}\right)\right] e^{ikr}$$

$$= -\frac{i\hbar}{m}(ik) + \frac{i\hbar |A|^2 4\pi}{m} \frac{2}{\alpha^2} \int_0^{\infty} r^3 e^{-2r^2/\alpha^2} = \dots = \frac{1}{m}\left(\hbar k + i \frac{2\hbar}{r_0}\right)$$

$v_{rad} = \frac{1}{m} \hbar k$

Thus: $\bar{J}(\bar{r},0) = e \frac{\hbar k}{m} \left(\frac{2}{\pi\alpha^2}\right)^{3/2} e^{-2r^2/\alpha^2} \hat{\rho}$

c) Current Density.

- Guessing the result from classical considerations

In general $\vec{J}(\vec{r},t) = e\,\vec{v}\cdot n(\vec{r},t)$

At $t=0$ $\vec{J}(\vec{r},0) = e\,\vec{v}\,n(\vec{r},0)$ depends only on the radial coordinate so

$$\vec{J}(\vec{r},0) \to J(r,0) = e\,\underbrace{v_{rad}}_{\text{radial vel.}}\,\underbrace{n(r,0)}_{\text{concentration.}}$$

i) $\psi(r,0) = A e^{-r^2/\alpha^2} e^{ikr} \neq A e^{ikr}$ (plane wave)

Let's make however a rough approx and take $k \to$ electron radial w. vector

so that $p_{rad} \simeq \hbar k$ or $v_{rad} = p_{rad}/m = \frac{\hbar}{m} k$

ii) Take concentration $n \to |\psi(r,0)|^2$ = electron prob. density $[1/\text{vol.}]$

Thus: $\boxed{J(r,0) \simeq e\cdot\frac{\hbar k}{m}\cdot|A|^2\,e^{-2r^2/\alpha^2}}$ Guess

Formal approach:

$$\vec{\nabla}_{\vec{r}} = \frac{\partial}{\partial r}\hat{\rho} + \frac{1}{r}\frac{\partial}{\partial \vartheta}\hat{\vartheta} + \frac{1}{r\sin\vartheta}\frac{\partial}{\partial \varphi}\hat{e}$$ (gradient / polar coord.s)

$$\vec{J}(\vec{r},t) \equiv \frac{i\hbar e}{2m_e}\left(\psi(\vec{r},t)\,\vec{\nabla}_{\vec{r}}\,\psi^*(\vec{r},t) - \psi^*(\vec{r},t)\,\vec{\nabla}_{\vec{r}}\,\psi(\vec{r},t)\right)$$

$$\vec{J}(\vec{r},0) = \frac{i\hbar e}{2m_e} \times \left\{ \psi(r,0)\,\underbrace{\partial_r \psi^*(r,0)}_{\left(-ik - 2\frac{r}{\alpha^2}\right)\psi^*(r,0)} - \psi^*(r,0)\,\underbrace{\partial_r \psi(r,0)}_{\left(ik - 2\frac{r}{\alpha^2}\right)\psi(r,0)} \right\}\hat{\rho}$$

$\psi(\vec{r},0)$ = has only radial comp. $= \psi(r,0)$

$$= \frac{i\hbar e}{2m_e}|A|^2 e^{-2r^2/\alpha^2} \times \left\{ -ik - \cancel{2\frac{r}{\alpha^2}} - ik + \cancel{2\frac{r}{\alpha^2}} \right\} = \frac{e\hbar|A|^2}{m}k\, e^{-2r^2/\alpha^2}\,\hat{\rho}$$

$$= e\left(\frac{\hbar k}{m_e}\right)\underbrace{\left(\frac{2}{\pi\alpha^2}\right)^{3/2} e^{-2r^2/\alpha^2}}\hat{\rho}$$

electron charge — analog of the classical radial velocity — prob. density

[charge] [space/time] [1/volume] → [charge / (time × surface)]

⇑

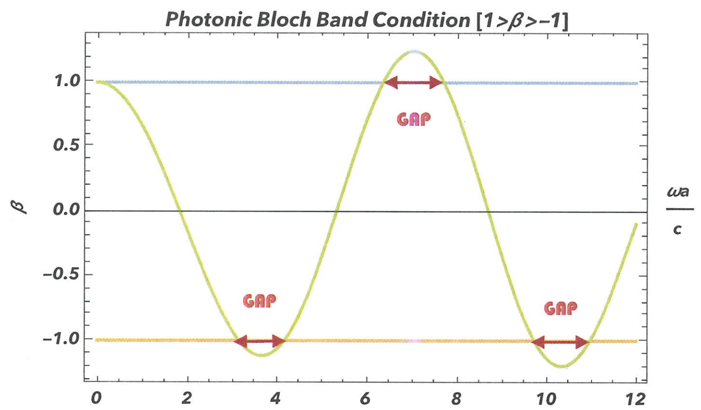
current density OK

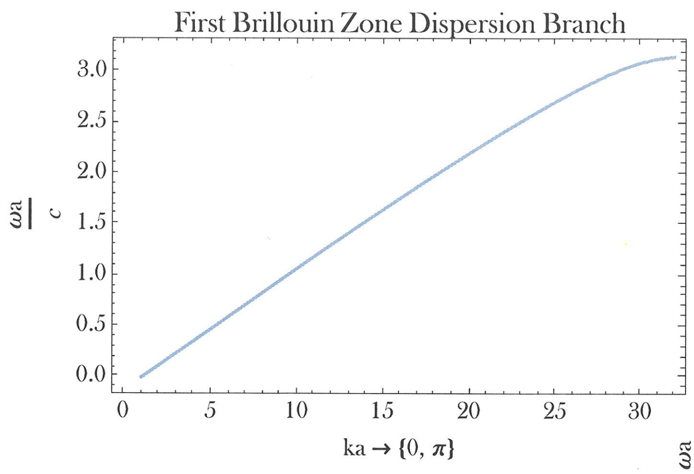
28. The reflection and transmission coefficient of a dielectric slab of thickness d are:

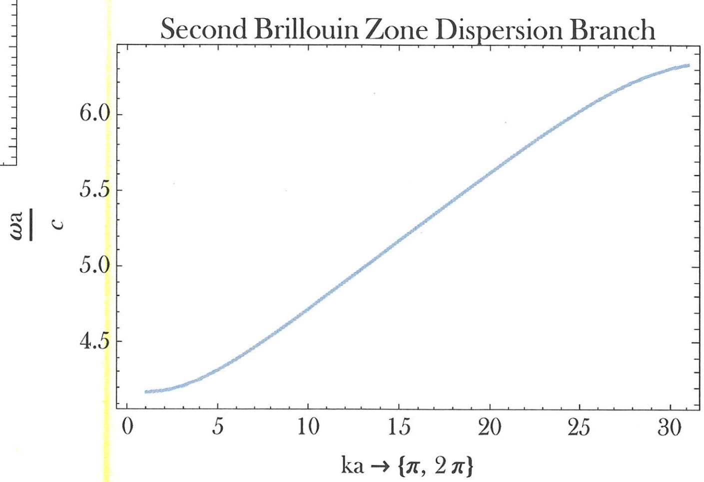
$$r = \frac{(n^2-1)\,(e^{2ikdn}-1)}{(n+1)^2-(n-1)^2 e^{2ikdn}} \qquad t = \frac{4n\,e^{ikdn}}{(n+1)^2-(n-1)^2 e^{2ikdn}}$$

A photonic crystal with n=2 (non absorbing) is made up of a periodic distribution of slabs of such a material whose periodicity and thickness are such that d/a=0.1.

a. Find the equation that describes the photonic band gap in terms of ωa/c.
b. Plot such an equation as a function of ωa/c.
c. Would an incident light beam with frequency such that ωa/c=3 e ωa/c=4 propagate or not.
d. Plot the dispersion bands for the 1st and 2nd Brillouin zone (positive Bloch wavevectors)







$$\boxed{\cos ka = \mathrm{Re}\left[e^{i\omega(a-d)/c} \frac{1}{t^*} \right] \equiv \beta(\omega)}$$

Photonic Band Dispersion Eq.

Incident freq.

$\uparrow$

$(k=\omega/c)$

$$t = \frac{4n e^{ikdn}}{(n+1)^2 - (n-1)^2 e^{2ikdn}} \qquad (n=2) \qquad t = \frac{8 \cdot e^{2ikd}}{9 - e^{4ikd}}$$

$$\beta(\omega) = \mathrm{Re}\left[\frac{9 - e^{4ikd}}{8} \cdot e^{ik(a-d)} \right] = \frac{1}{8} \times \left\{ 9 \cos k(a-d) - \cos k(a+3d) \right\}$$

$$= \frac{1}{8} 9 \cos \frac{\omega a}{c} \left(1 - \frac{d}{a}\right) - \frac{1}{8} \cos \frac{\omega a}{c} \left(1 + 3\frac{d}{a}\right)$$

$$\frac{d}{a} = 0.1$$

$$\beta\left(\frac{\omega a}{c}\right) = \frac{9}{8} \cos\left[0.9 \frac{\omega a}{c}\right] - \frac{1}{8} \cos\left[1.3 \frac{\omega a}{c}\right]$$

Band-gap condition: $\beta < -1$ & $\beta > 1$ $\qquad \frac{\omega a}{c} \equiv x$ (No dimension)

a.) $\frac{9}{8} \cos[0.9x] - \frac{1}{8} \cos[1.3x] > 1$

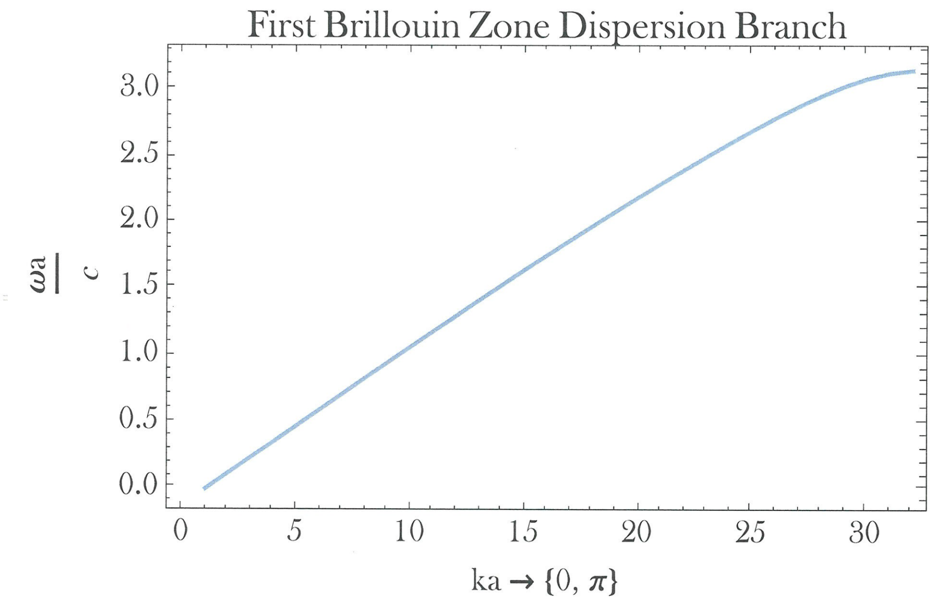
$\qquad$ " $\qquad\qquad$ " $\qquad < 1$

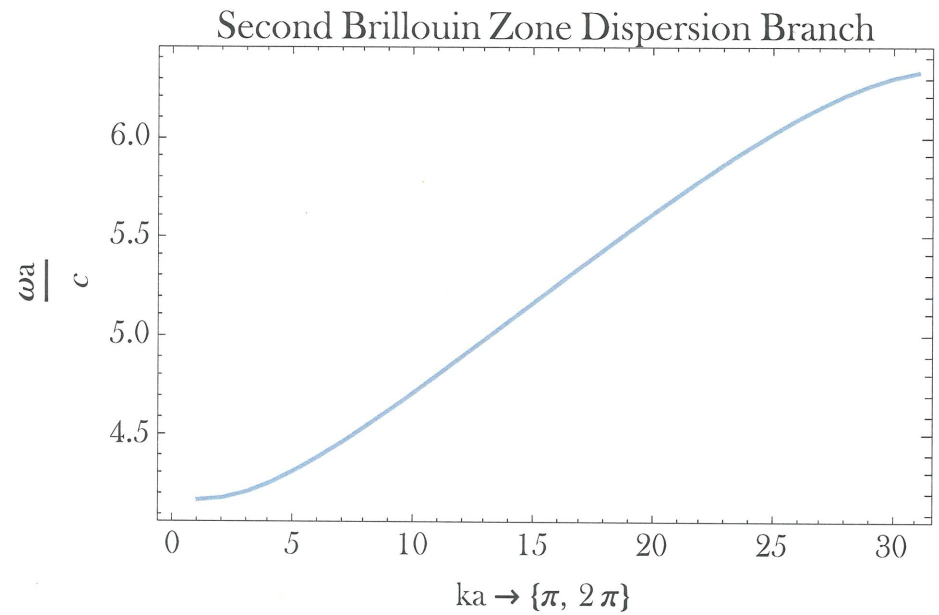
c.) $\beta(x=3) = -0.92$ (Propagating Mode)

$\beta(x=4) = -1.067$ (Band-gap Mode)

b.) See plots.

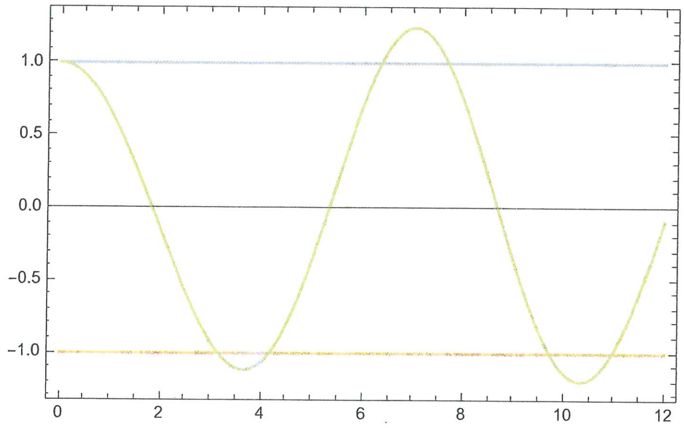
d.) See plots & program.


First Brillouin Zone Dispersion Branch
ωa / c
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
5
10
15
20
25
30
ka → {0, π}

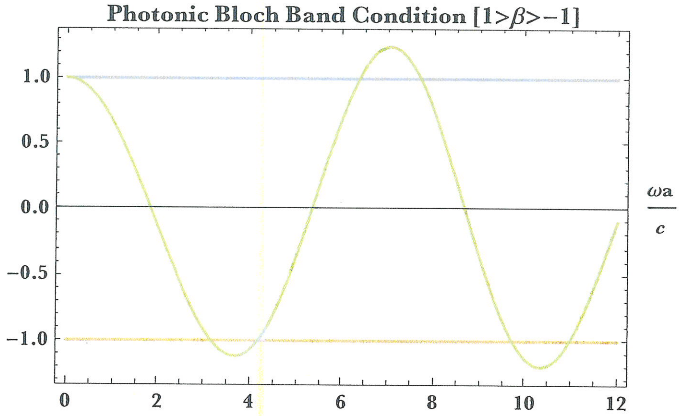

Second Brillouin Zone Dispersion Branch
ωa / c
6.0
5.5
5.0
4.5
0
5
10
15
20
25
30
ka → {π, 2 π}

```
In[9]:= β = 9/8 Cos[0.9 w] - 1/8 Cos[1.3 w];
        β /. {w → 3}
        β /. {w → 4}
Out[10]= -0.92634
Out[11]= -1.06742
```

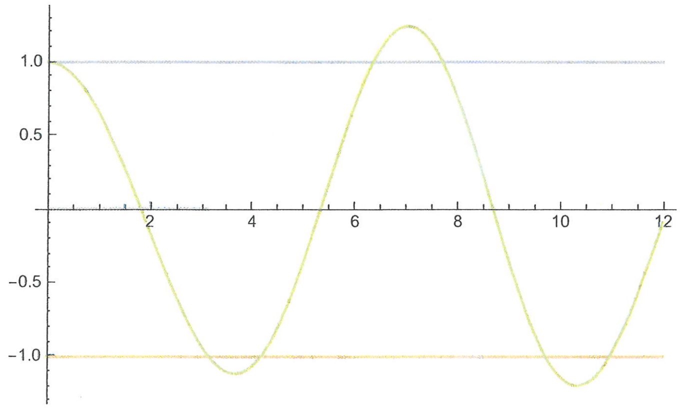
```
In[15]:= Plot[{1, -1, β}, {w, 0, 12}, Frame → True]
```



```
Show[%16, AxesLabel → {HoldForm[ωa/c], HoldForm[β]},
  PlotLabel → HoldForm[Photonic Bloch Band Condition "[1>β>-1]"],
  LabelStyle → {FontFamily → "Baskerville", 11, GrayLevel[0], Bold}]
```

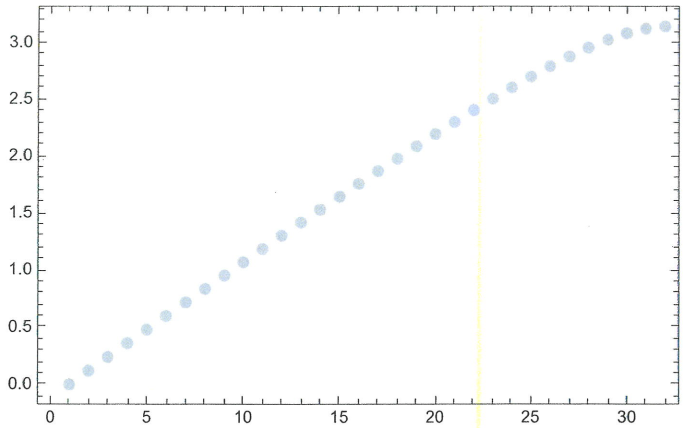


```
Show[
  Plot[{1, -1, 9/8 Cos[0.9 w] - 1/8 Cos[1.3 w]}, {w, 0, 12}], Plot[0 × 8 Cos[k], {k, 0, π}]
]
```



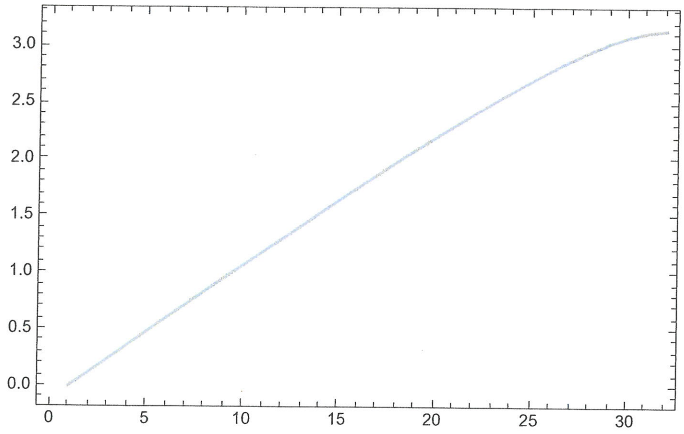

```
list1 = Flatten[
    Table[FindRoot[9/8 Cos[0.9 w] - 1/8 Cos[1.3 w] == Cos[k], {w, 1.5}], {k, 0, π, .1}]];
Table[list1[[j]][[2]], {j, 1, 32}]
ListPlot[%, Frame → True]
```

{−2.28222 × 10^{-9}, 0.119512, 0.238957, 0.35827, 0.477385, 0.596237, 0.714761, 0.832893, 0.950571, 1.06773, 1.18431, 1.30025, 1.41547, 1.52991, 1.6435, 1.75614, 1.86776, 1.97823, 2.08743, 2.1952, 2.30133, 2.40556, 2.50755, 2.60684, 2.70281, 2.79457, 2.8809, 2.96007, 3.02972, 3.08668, 3.1272, 3.14763}



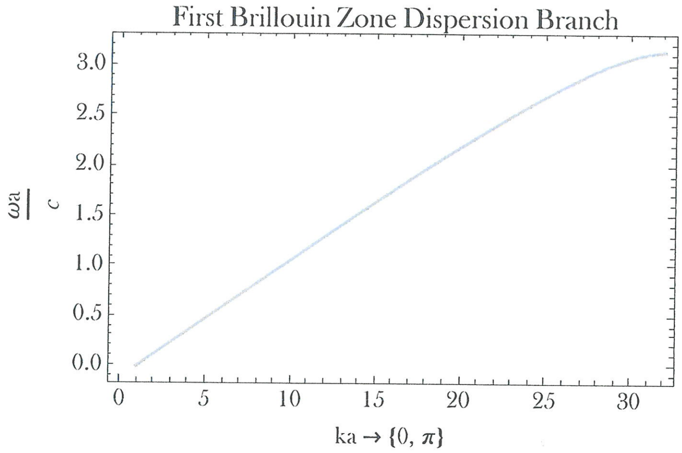
In[162]:= ListLinePlot[%%, Frame -> True]

Out[162]=



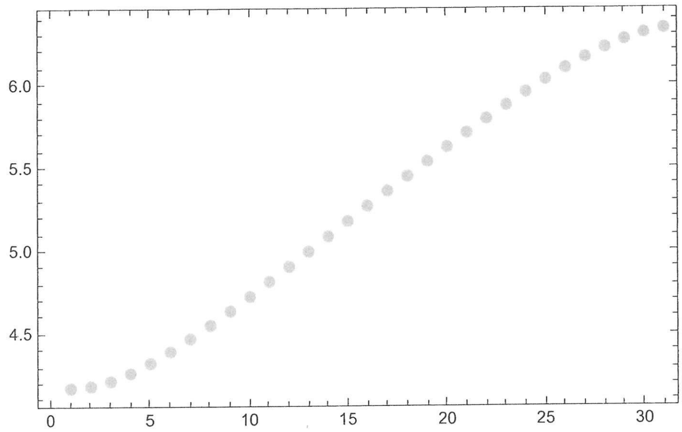
In[168]:= Show[%166, PlotLabel → HoldForm[First Brillouin Zone Dispersion Branch],
LabelStyle → {FontFamily → "Baskerville Old Face", 13, GrayLevel[0], Bold}]

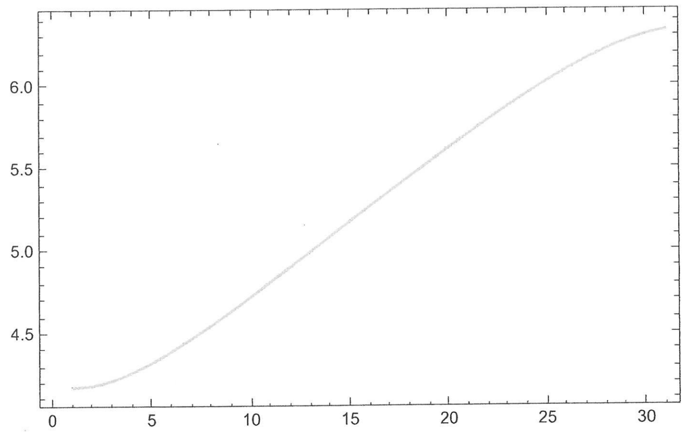
Out[168]=



```
list2 = Flatten[Table[
    FindRoot[9/8 Cos[0.9 w] - 1/8 Cos[1.3 w] == Cos[k], {w, 5.1}], {k, π, 2 π, .1}]];
Table[list2[[j]][[2]], {j, 1, 31}]
ListPlot[%, Frame -> True]
ListLinePlot[%%, Frame → True]
```

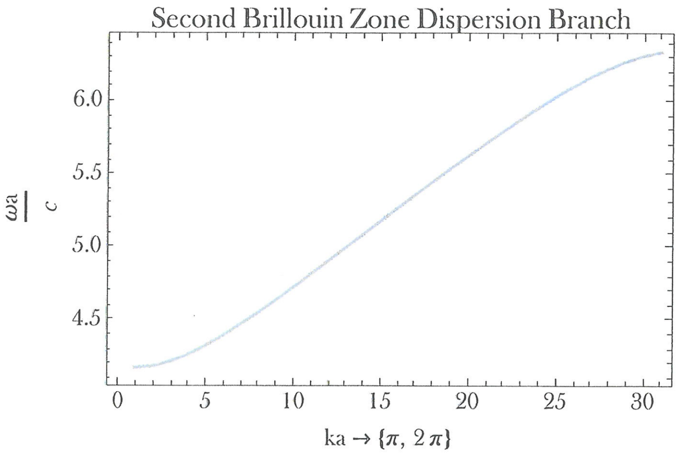
```
{4.17553, 4.18621, 4.21698, 4.26457, 4.32515, 4.39527, 4.4722,
 4.55397, 4.63914, 4.72668, 4.81584, 4.90607, 4.99693, 5.0881, 5.17927,
 5.2702, 5.36064, 5.45038, 5.53915, 5.62669, 5.71267, 5.79673, 5.87841,
 5.95713, 6.03219, 6.10269, 6.16752, 6.22532, 6.27449, 6.31327, 6.33992}
```

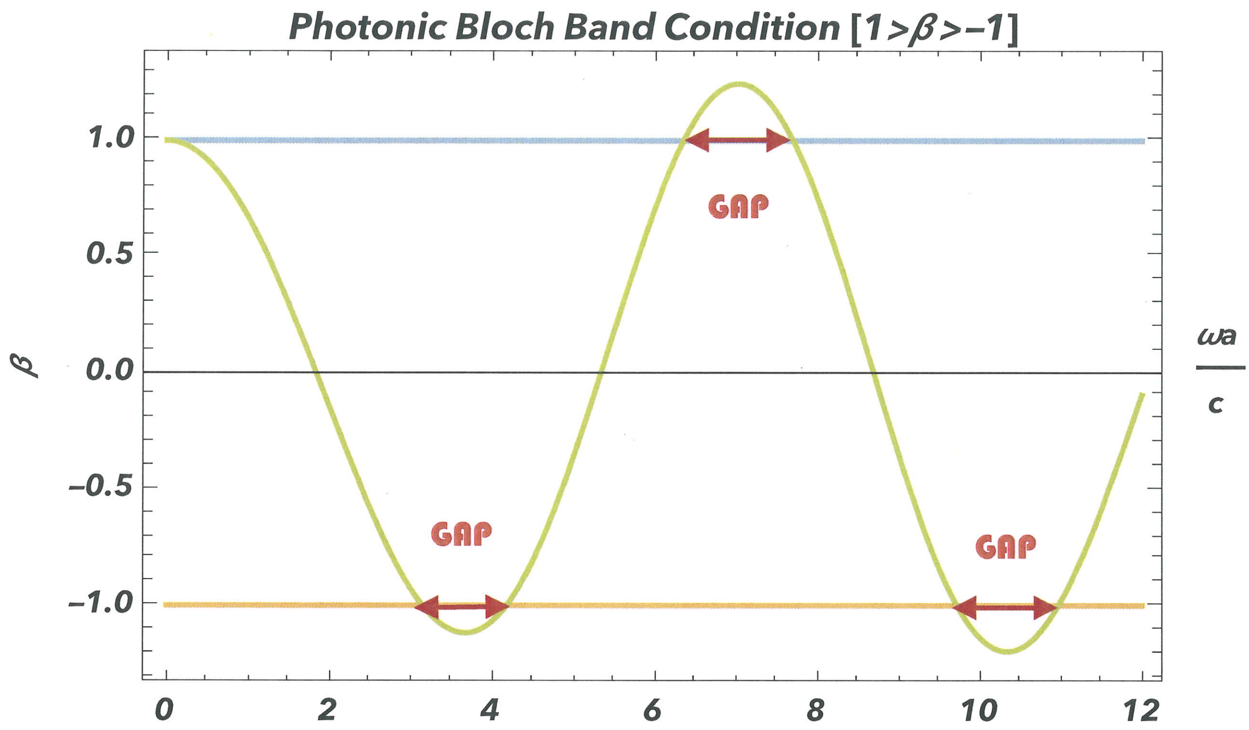




In[178]:=
```
Show[%177, FrameLabel → {{HoldForm[ωa/c], None}, {HoldForm[ka → {π, 2 π}], None}},
  PlotLabel → HoldForm[Second Brillouin Zone Dispersion Branch]]
```

Out[178]=




Photonic Bloch Band Condition [1>β>−1]
1.0
0.5
0.0
−0.5
−1.0
β
0
2
4
6
8
10
12
ωa/c
GAP
GAP
GAP

A charge q may tunnel from a metal through the application of a suitable (constant) external electric field ε. After the application of the electric field $\mathscr{E}$ the potential at the metal surface taken at $x = a$ reads as (see class notes)

$$V(x) = \Phi + E_F - q\mathscr{E}(x - a)$$

Assuming that the tunneling charge originates from a single-electronic state, estimate the field strength ε (volt/cm) needed to draw (tunneling) current densities of the order of mA/cm^2 from a potassium (K) sample surface.

Use definition: $\frac{J_{out}}{J_{in}} = T$ $\qquad T = e^{-\frac{4}{3}\frac{\sqrt{2m}}{\hbar}\frac{\Phi^{3/2}}{|e|\mathcal{E}}}$ (in class)

$J_{in} = |e|\frac{N}{V}v$ $\qquad$ Typical values for k: $\frac{N}{V} \sim \frac{1.4\times10^{22}}{cm^3}$ $\qquad v \sim v_F = 0.86\times10^{8}\,\frac{cm}{sec.}$

$$= 1.6\times10^{-19}C\ \frac{1.4\times10^{22}}{10^{-6}m^3}\ 0.86\times10^{6}\frac{m}{s} = \left[\frac{A}{m^2}\right]\ 1.9\times10^{15}$$

$$J_{out} = \frac{mA}{cm^2} = \frac{10^{-3}A}{10^{-4}cm^2} = 10\ \frac{A}{cm^2}$$

$\Phi \sim eV$

$$\frac{J_{out}}{J_{in}} = \frac{10\ A/m^2}{1.9\times10^{15}\ A/m^2} = e^{-\frac{4}{3}\frac{\sqrt{2mc^2}}{\hbar c}\frac{\Phi^{3/2}}{|e|\mathcal{E}}}$$

or:

$$-32.89 \simeq -\frac{4}{3}\ \frac{\sqrt{2\times0.5\times10^{6}eV}}{1973\,eV\times10^{-10}m}\ \frac{(1\,eV)^{3/2}}{1.6\times10^{-19}C\ \mathcal{E}}$$

$1.6\times10^{-19}J = 1.6\times10^{-19}\ C\times V$

$$= -\frac{4}{3}\ \frac{10^{3}\ eV^{2}}{1973\ eV\ 1.6\times10^{-29}\ m\,C\ \mathcal{E}}$$

$$= -\frac{4}{3}\times\frac{10^{3}\times\cancel{1.6}\times10^{-19}}{1973\times\cancel{1.6}\times10^{-29}\ \mathcal{E}}(V/m) \cong -6.7\times10^{9}\ \frac{V/m}{\mathcal{E}}$$

or

$$\mathcal{E} \sim 2\times10^{8}\ \frac{V}{m} = 2\times10^{6}\ \frac{V}{cm}$$

(*)

That's a rough estimate as it assumes that <u>all</u> electrons take part into the tunneling process and that all electrons have <u>same velocity</u> (v_F).