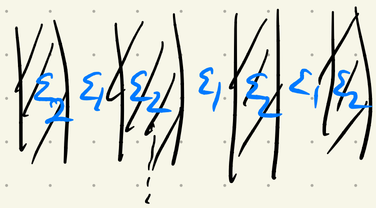
The origin of gap in 1d-periodic

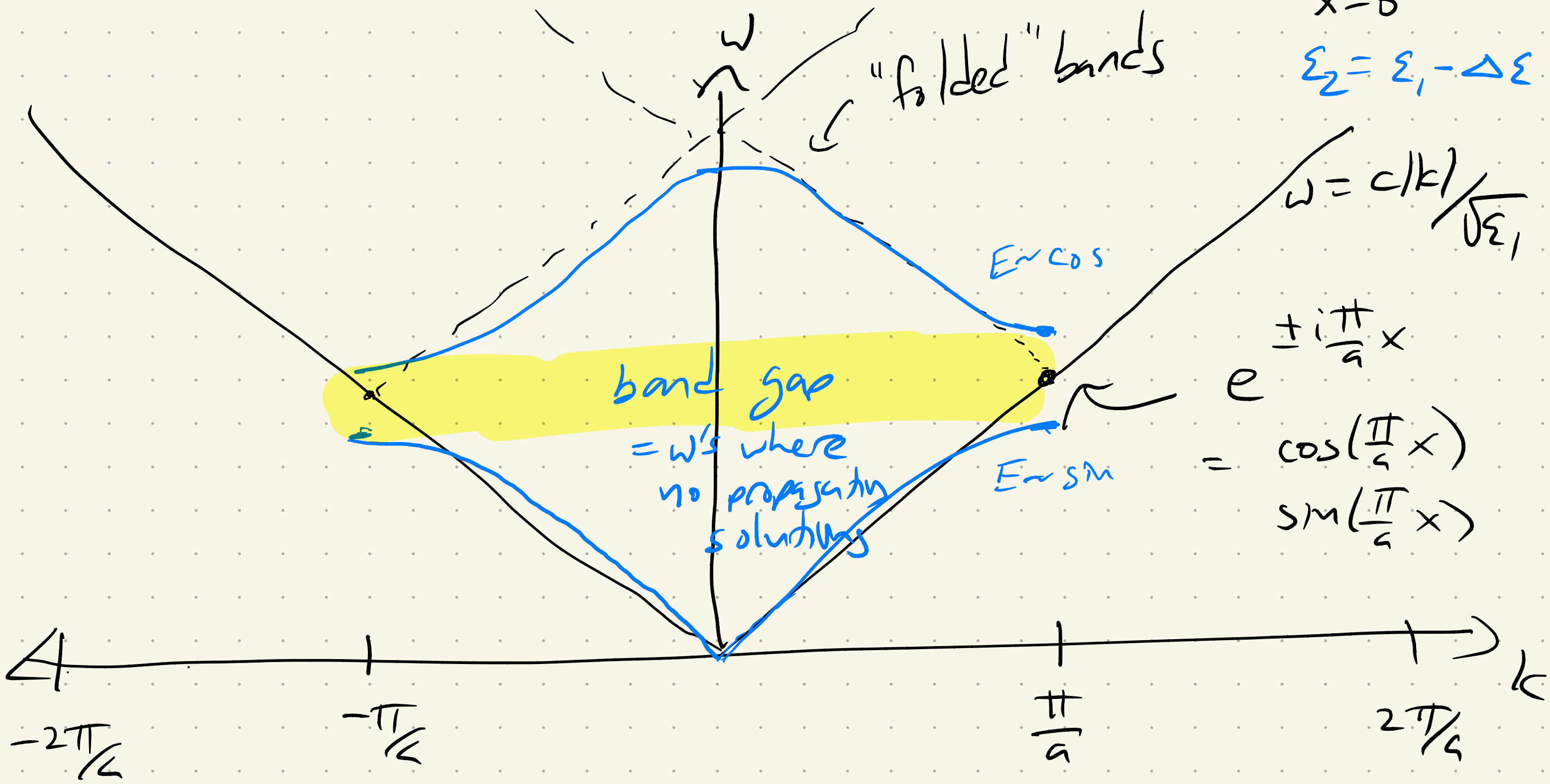
start with uniform $\boxed{\varepsilon = \varepsilon_1}$

period a



$\varepsilon_2 = \varepsilon_1 - \Delta\varepsilon$

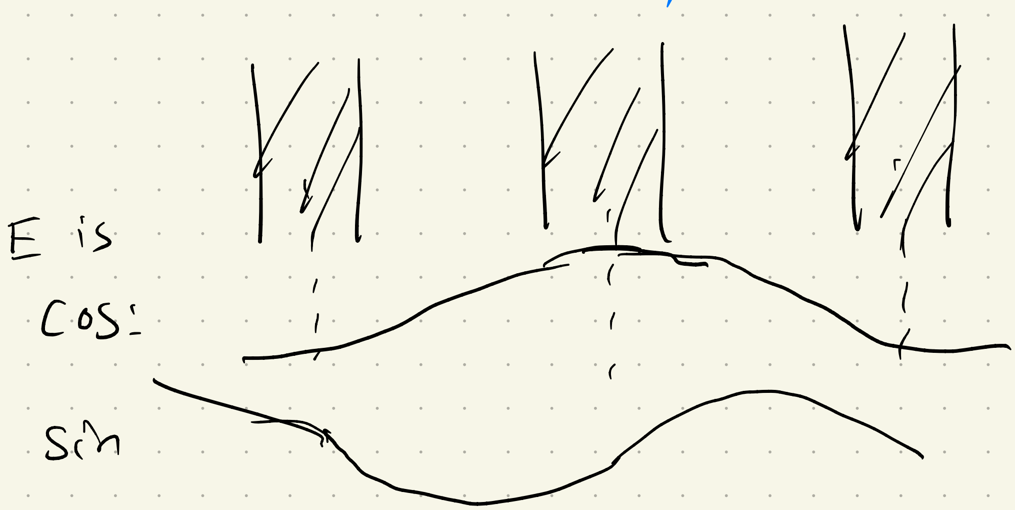
→ turn on periodic modulation
($\Delta\varepsilon$ increase continuously)



$e^{\pm i \frac{\pi}{a} x} = \cos(\frac{\pi}{a} x)$, $\sin(\frac{\pi}{a} x)$

Then turn on periodicity:

higher ε = lower ω



peaked in ε_2 < peaked in ε_1

Quantify this using perturbation theory

- perturbation theory: solve one problem, approximately solve nearby problems
  - insight into weak effects, small change
  - numerically, computers are bad at small effects (big contrast in scales)

Eigenvalue perturbation theory

given Hermitian eigenproblem $\hat{O} u = \lambda u$

$\hat{O} = \hat{O}^{+}$

$\Rightarrow$ approximately solve perturbed problem

$$(\hat{O} + \Delta \hat{O})(u + \Delta u) = (\lambda + \Delta\lambda)(u + \Delta u)$$

for small $\Delta \hat{O}$ (need not be Hermitian)

- imagine $\Delta\hat{O}$ proportional to small parameter δ, Taylor expand u, λ in powers of δ, collect terms order by order:

$$u + \Delta u = \underset{\sim\delta^0}{u^{(0)}} + \underset{\sim\delta^1}{u^{(1)}} + \underset{\sim\delta^2}{u^{(2)}} + \cdots$$

$$\lambda + \Delta\lambda = \lambda^{(0)} + \lambda^{(1)} + \lambda^{(2)} + \cdots$$

Plug in:

$$(\hat{O} + \Delta\hat{O})(u^{(0)} + u^{(1)} + \cdots)$$

$$= (\lambda^{(0)} + \lambda^{(1)} + \cdots)(u^{(0)} + u^{(1)} + \cdots)$$

δ^0 terms: $\hat{O} u^{(0)} = \lambda^{(0)} u^{(0)}$

(unperturbed solution)

δ^1 terms: $\hat{O} u^{(1)} + \Delta\hat{O} u^{(0)} = \lambda^{(0)} u^{(1)} + \lambda^{(1)} u^{(0)}$

$\Longrightarrow$ solve for $\lambda^{(1)}$ = 1st order correction to λ

trick: $\langle u^{(0)}, \hat{O} u^{(1)}\rangle + \langle u^{(0)}, \Delta\hat{O} u^{(0)}\rangle$

$$= \lambda^{(0)}\langle u^{(0)}, u^{(1)}\rangle + \lambda^{(1)}\langle u^{(0)}, u^{(0)}\rangle$$

Hermitian: $\cancel{\langle \hat{O} u^{(0)}, u^{(1)} \rangle = \underset{\text{real}}{\lambda^{(0)}} \langle u^{(0)}, u^{(1)} \rangle}$

trick: $\underline{\langle u^{(0)}, \hat{O} u^{(1)} \rangle} + \langle u^{(0)}, \Delta\hat{O} u^{(0)} \rangle$

$= \cancel{\underline{\lambda^{(0)} \langle u^{(0)}, u^{(1)} \rangle}} + \lambda^{(1)} \langle u^{(0)}, u^{(0)} \rangle$

all $u^{(1)}$ terms cancel!

$$\Rightarrow \boxed{\lambda^{(1)} = \Delta\lambda \text{ to } 1^{st} \text{ order} = \frac{\langle u^{(0)}, \Delta\hat{O} u^{(0)} \rangle}{\langle u^{(0)}, u^{(0)} \rangle}}$$

Application to Maxwell:

$$\nabla\times\tfrac{1}{\varepsilon}\nabla\times H = \hat{\Theta} H = \omega^2 H$$

$$\Rightarrow \text{given } \Delta\varepsilon \Rightarrow \Delta\hat{\Theta} = \nabla\times \Delta\left(\tfrac{1}{\varepsilon}\right) \nabla\times$$

$$\Delta\left(\tfrac{1}{\varepsilon}\right) = \frac{1}{\varepsilon+\Delta\varepsilon} - \frac{1}{\varepsilon}$$

$$\Delta(\omega^2) = \frac{\langle H, \Delta\hat{\Theta} H \rangle}{\langle H, H \rangle} = \frac{\int H\cdot\nabla\times\Delta\left(\tfrac{1}{\varepsilon}\right)\nabla\times H}{\int |H|^2}$$

int by parts

$$= \frac{\int \Delta\left(\tfrac{1}{\varepsilon}\right) |\nabla\times H|^2}{\int |H|^2}$$

Further simplifications:

numerator: $\int \Delta\left(\frac{1}{\varepsilon}\right) |\underbrace{\nabla\times H}_{= -i\omega\varepsilon E}|^2 = \omega^2 \int \underbrace{\Delta\left(\frac{1}{\varepsilon}\right)}_{=\frac{1}{\varepsilon+\Delta\varepsilon}-\frac{1}{\varepsilon}} \cancel{\varepsilon^2} |E|^2$

$$= -\omega^2 \int \Delta\varepsilon |E|^2$$

$$= -\frac{\Delta\varepsilon}{\cancel{\varepsilon^2}} + \cancel{O(\Delta\varepsilon^2)}$$

only keeping 1st order terms

lemma: in a time-Harmonic field, H and E store same time-average energy

denominator:

$$\int |H|^2$$

$$= \int H^* \cdot \left(\frac{1}{i\omega} \nabla \times E\right) = \int (\underbrace{\nabla\times H}_{=-i\omega\varepsilon E})^* \cdot \frac{E}{i\omega}$$

int by parts

$$= \int \varepsilon |E|^2$$

$$\Delta(\omega^2) = (\omega + \Delta\omega)^2 - \omega^2$$

$$= 2\omega\Delta\omega + \cancel{\Delta\omega^2}$$

drop (2nd order)

putting it all together:

$$\boxed{\Delta\omega = -\frac{\omega}{2}\frac{\int \Delta\varepsilon|E|^2}{\int \varepsilon|E|^2}}$$

notice: $\Delta\varepsilon > 0 \Rightarrow \Delta\omega < 0$ (to 1st order)
(ω "pulled down")

$\Delta\omega$ related to how much $|E|^2$ we have in $\Delta\varepsilon$ region

nice intuition about effect of perturbations

more precise: suppose

constant $\Delta\varepsilon, \varepsilon$ $\quad \Delta\varepsilon = 0$

fractional change in ω $\to \frac{\Delta\omega}{\omega} = -\frac{\omega}{2}\frac{\frac{\Delta\varepsilon}{\varepsilon}\int_{\Delta\varepsilon\neq 0} \varepsilon|E|^2}{\int \varepsilon|E|^2}$

$$= -\frac{1}{2}\cdot\underbrace{\frac{\Delta\varepsilon}{\varepsilon}}_{\text{fractional change in }\varepsilon}\left(\text{fraction of }\varepsilon|E|^2\text{ in perturbation}\right)$$

Another nice application:

$\varepsilon = \varepsilon' + i\varepsilon''$
real part   imag. part

absorption loss in low-loss material = small imaginary part added to ε

$(\operatorname{Im}\varepsilon \ll \operatorname{Re}\varepsilon)$

decaying solutions

$= \text{non-Hermitian perturbation } \Delta\varepsilon$
$= i\varepsilon''$

(passivity: $\omega \operatorname{Im}\hat{\chi} = \omega \operatorname{Im}\varepsilon$
$= \omega\varepsilon'' \geq 0$
$\Rightarrow \varepsilon''$ = same sign as ω)

$$\Longrightarrow \Delta\omega = -\frac{\omega}{2}\frac{i\varepsilon''}{\varepsilon'}$$ (fraction of $\varepsilon|E|^2$ in absorbing material)

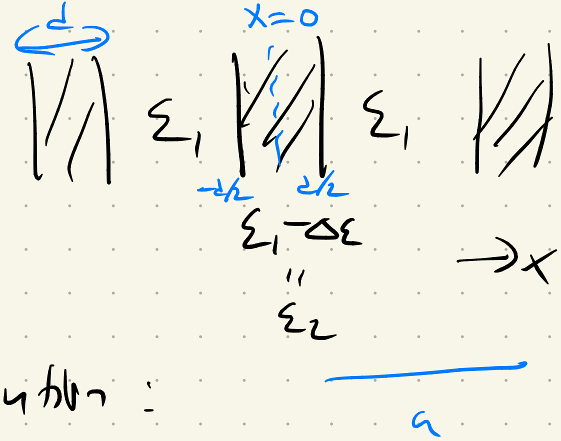
= imaginary change in ω with <u>negative</u> imaginary part

$\Delta\omega = -i\alpha$
$(\alpha > 0)$

$$e^{-i\omega t} \longrightarrow e^{-i(\omega+\Delta\omega)t}$$
$$= e^{-i\omega t - \alpha t}$$

exponentially decaying in time!

Back to band gaps:



unperturbed ($\Delta\varepsilon = 0$) solution:

$$E_z(x) = \cos\left(\frac{\pi x}{a}\right)$$

or

$$\sin\left(\frac{\pi x}{a}\right)$$

$$\omega = \frac{k}{\sqrt{\varepsilon_1}} = \frac{\pi}{a\sqrt{\varepsilon_1}}$$

$$\frac{\Delta\omega_{\cos}}{\omega} = +\frac{1}{\cancel{2}} \frac{\cancel{2}\int_0^{d/2} (\cancel{+}\Delta\varepsilon)\cos^2\left(\frac{\pi x}{a}\right)dx}{\int_{-a/2}^{a/2} \varepsilon_1 \cos^2\left(\frac{\pi x}{a}\right)dx}$$

'' $\dfrac{1+\cos\left(\frac{2\pi x}{a}\right)}{\cancel{2}}$

'' $\dfrac{1+\cos\left(\frac{2\pi x}{a}\right)}{\cancel{2}}$ integrates to 0

$$> \quad = \frac{\Delta\varepsilon}{\varepsilon_1 a}\left[\frac{d}{2} + \frac{a}{2\pi}\sin\left(\frac{\pi d}{a}\right)\right]$$

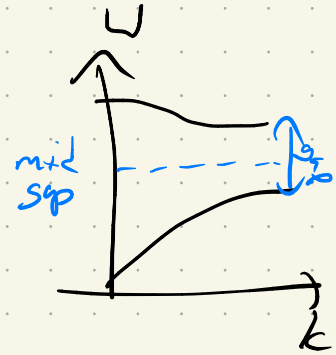
$$\frac{\Delta\omega_{\sin}}{\omega} = \ldots\ldots = \frac{\Delta\varepsilon}{\varepsilon_1 a}\left[\frac{d}{2} - \frac{a}{2\pi}\sin\left(\frac{\pi d}{a}\right)\right]$$

similar, except $\sin^2\left(\frac{\pi x}{a}\right)$

$$= \frac{1-\cos\left(\frac{2\pi x}{a}\right)}{2}$$

gap: $\Delta\omega_{\cos} - \Delta\omega_{\sin} = \omega \dfrac{\Delta\varepsilon}{\varepsilon} \dfrac{\sin\left(\frac{\pi d}{a}\right)}{\pi}$

non-dimensionalize:



$$\text{fractional gap} = \frac{\text{gap}}{\text{mid-gap}}$$

$$= \frac{\omega \dfrac{\Delta\varepsilon}{\varepsilon} \dfrac{\sin\left(\frac{\pi d}{a}\right)}{\pi}}{\omega + \dfrac{\Delta\omega_{\cos} + \Delta\omega_{\sin}}{2}} \quad \sim \Delta\varepsilon$$

$$= \frac{\omega \frac{\Delta\varepsilon}{\varepsilon} \frac{\sin(\pi d/a)}{\pi}}{\omega} + O(\Delta\varepsilon)^2$$

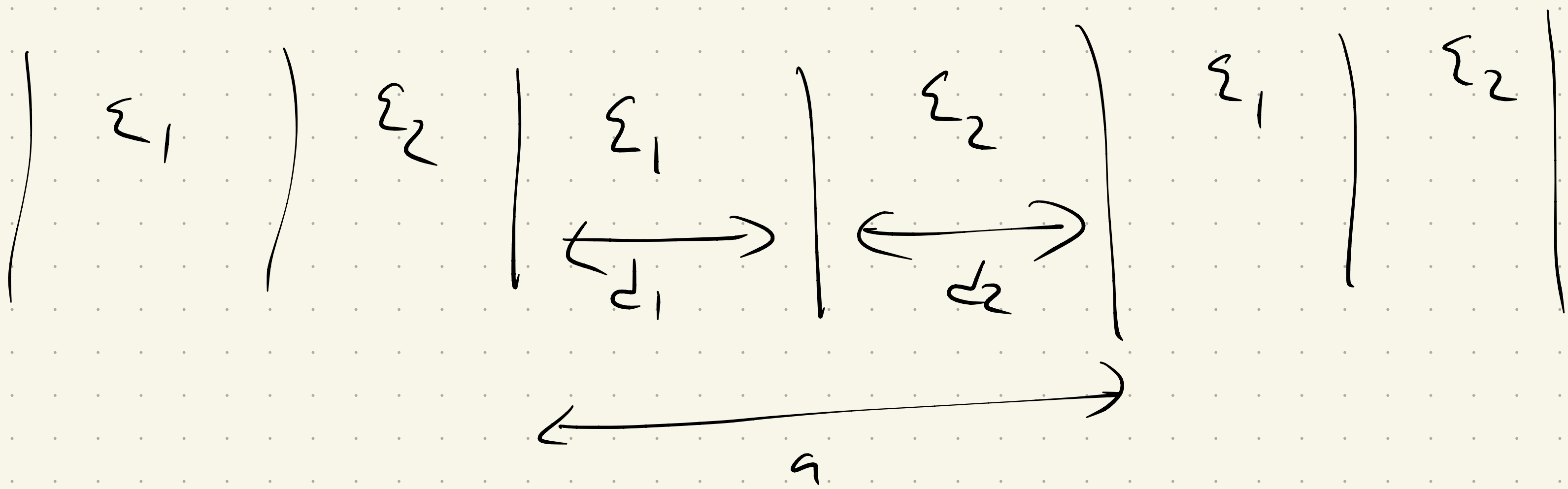
$$= \boxed{\frac{\Delta\varepsilon}{\varepsilon} \frac{\sin\left(\frac{\pi d}{a}\right)}{\pi}} + O(\Delta\varepsilon)$$

Note: proportional to $\frac{\Delta\varepsilon}{\varepsilon}$ (to 1st order)

maximum (for small $\Delta\varepsilon$) for $d = a/2$

- More generally:

  in 1d, can solve everything analytically for arbitrary $\Delta\varepsilon$, and it turns out that max fractional gap is for "quarter-wave stack"



quarter wave stack:

$$d_1\sqrt{\varepsilon_1} = d_2\sqrt{\varepsilon_2}$$

(P. Yeh: Optical Waves in Layered Media)
all 1d formulas

* Caveat: in general if you have degenerate eigenvals (like cos, sin sols)

procedure to find right linear combinations of unperturbed sols ⟸ you have to use "degenerate perturbation theory"

suppose

$$\hat{O} u_1 = \lambda u_1$$
$$\hat{O} u_2 = \lambda u_2$$

} degenerate, linearly independent u_1, u_2

$\Rightarrow$ perturbation theory:

$$u + \delta u = \underbrace{u^{(0)}}_{} + u^{(1)} + \ldots$$

In our case: picked right linear combination using $x=0$ mirror symmetry

$\Rightarrow$ even/odd solutions

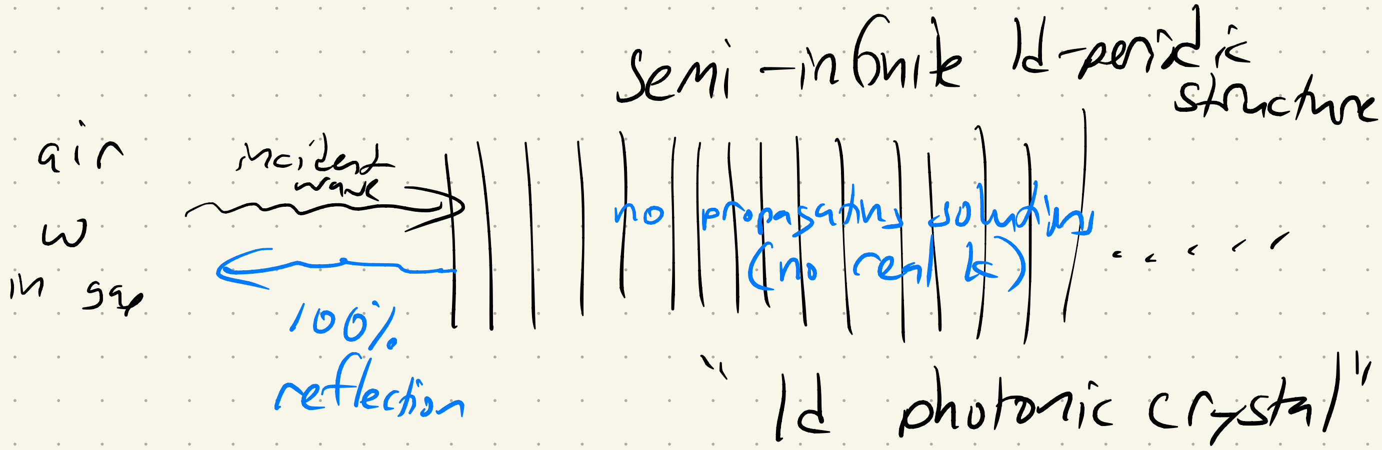
$\Rightarrow$ $\boxed{\cos\left(\frac{\pi x}{L}\right), \sin\left(\frac{\pi x}{L}\right)}$

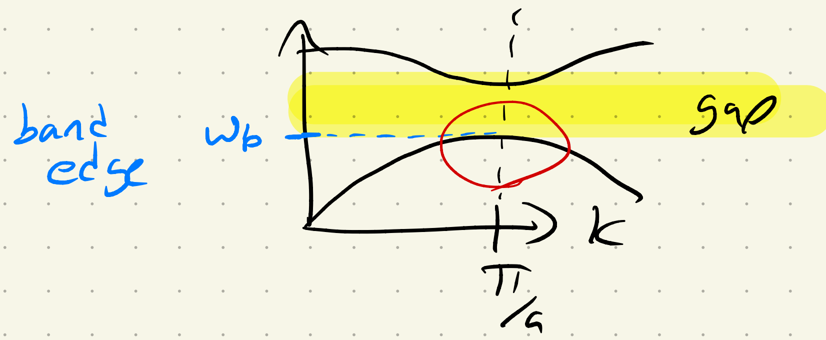
and not $e^{\pm i\frac{\pi}{L}x}$

problem: $u^{(0)}$ can be any linear combination of u_1, u_2

$\Rightarrow$ which one is the correct one?

Some consequences of gaps:





More precisely, what is field in crystal at ω in gap?

Look slightly within gap: $\omega = \omega_b + \delta\omega$ for small $|\delta\omega| \ll \omega_b$

$\Rightarrow$ Taylor expand $\omega(k)$ around $k = \pi/a$:

$$\omega(k) \approx \omega_b + \underset{\left(\frac{d\omega}{dk}=0 \text{ at } \frac{\pi}{a}\right)}{0} - \underset{-\frac{1}{2}\frac{d^2\omega}{dk^2}\Big|_{\pi/a}}{\underbrace{\alpha}}\left(k - \frac{\pi}{a}\right)^2$$

$\Rightarrow$ solve for $k(\omega_b + \delta\omega)$

$$\omega(k) \approx \omega_b + \underbrace{0}_{\left(\frac{d\omega}{dk}=0 \text{ at } \frac{\pi}{a}\right)} - \underbrace{\alpha}_{-\frac{1}{2}\frac{d^2\omega}{dk^2}\Big|_{\pi/a}}\left(k-\frac{\pi}{a}\right)^2$$

$\Rightarrow$ solve for $k(\omega_b + \delta\omega)$

$$k(\omega) = \sqrt{\frac{\omega_b - \omega}{\alpha}} + \frac{\pi}{a}$$

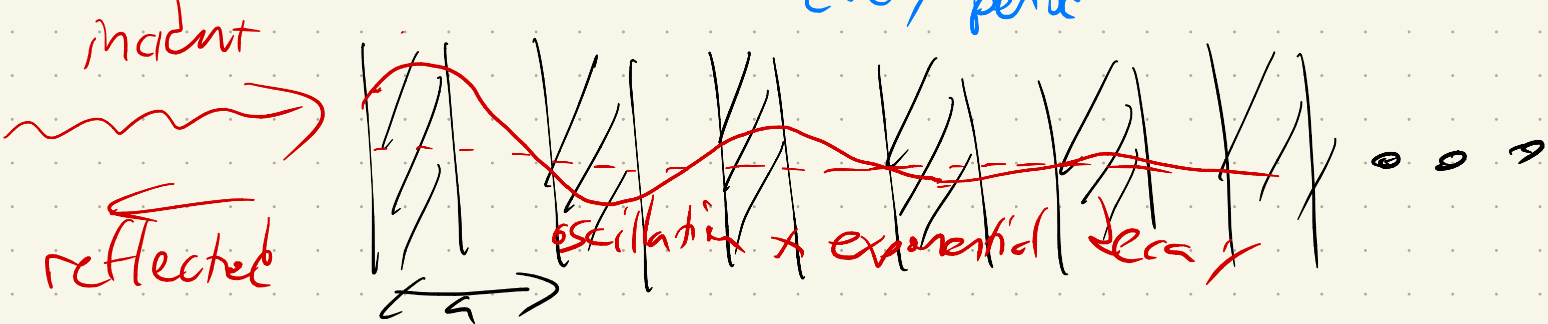
$\Rightarrow$ at $\omega = \omega_b + \delta\omega$,

$$k = i\sqrt{\frac{\delta\omega}{\alpha}} + \frac{\pi}{a}$$

$\Rightarrow$ solutions $e^{ikx} \cdot (\text{periodic})$

$$= \underbrace{e^{i\frac{\pi}{a}x}}_{\text{oscillates in sign every period}} \; \underbrace{e^{-\sqrt{\frac{\delta\omega}{\alpha}}}}_{\text{exponentially decaying}} (\text{periodic})$$

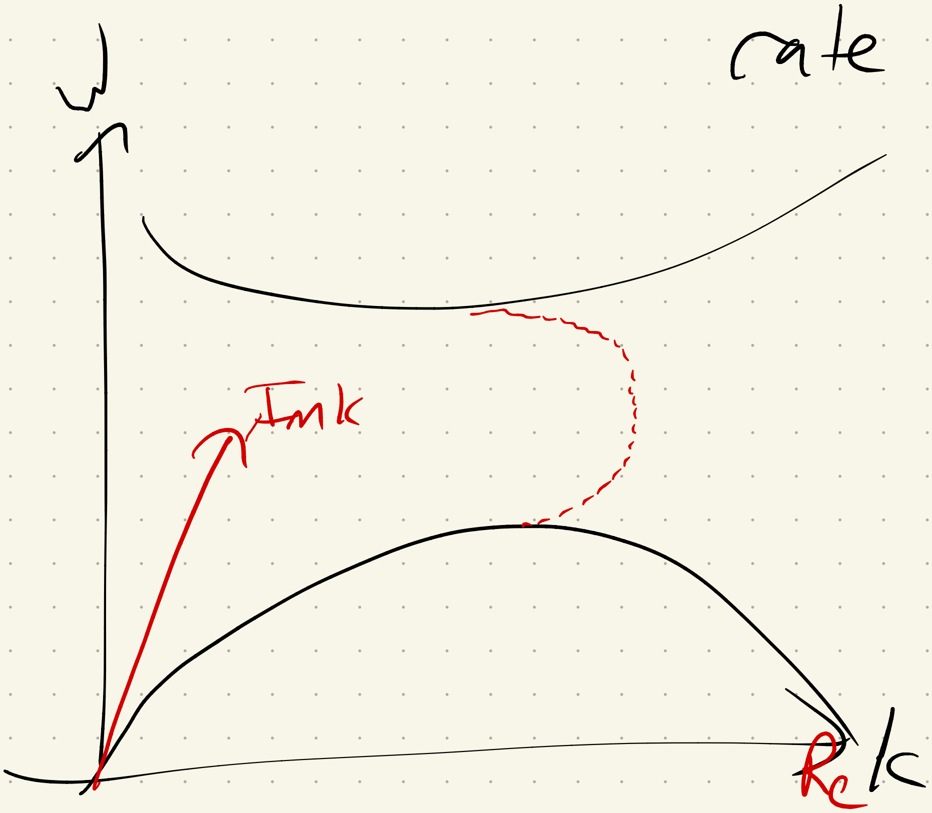
decay rate $\sim \sqrt{\omega - \omega_b}$

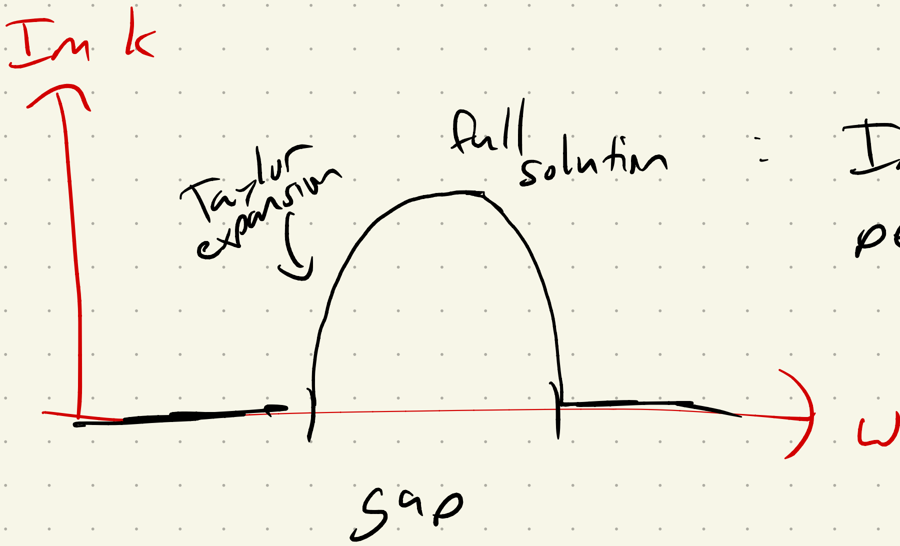


Carrolary: larger gap $\Rightarrow$

larger $\sqrt{\frac{\delta U}{w_b}}$

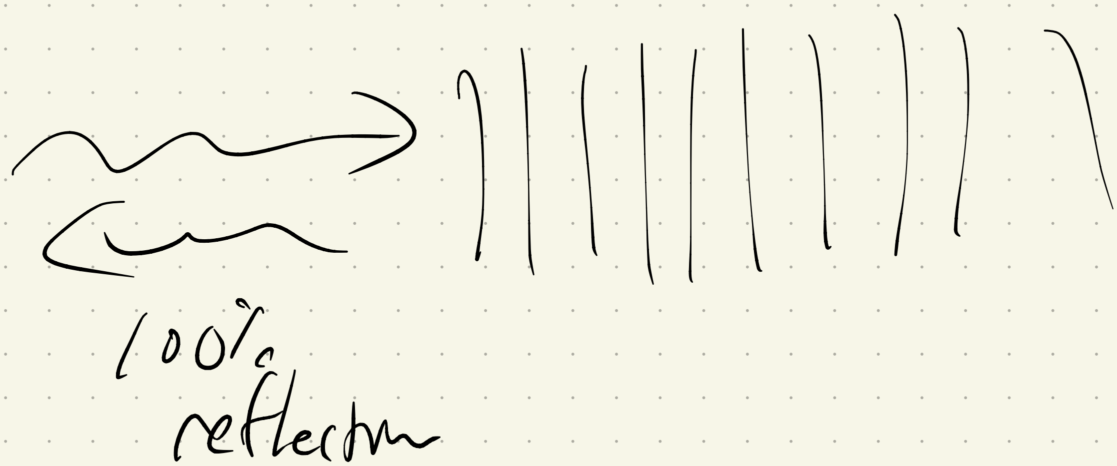
$\Rightarrow$ faster decay rate = stronger confinement





: Im k peaks ~ midgap ω

"Bragg mirror"



Trap light in "Fabry-Perot" cavity

$\Rightarrow$ resonant effects

to be continued