Density of States + Local Density of States
(DOS) (LDOS)

* Gives way of talking about ~~eigenfunctions~~ eigenvalues + spectrum that generalizes easily to finite periodic systems surrounded by ∞ space, to ~~to~~ lossy systems, to irregular/aperiodic cases in general

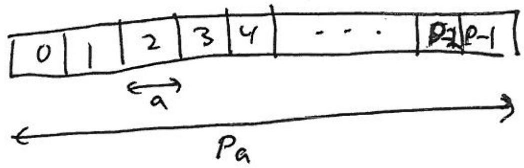
— essential tool for thinking about resonances

* Simplest case: assume finite domain ("universe lives in a box"), Hermitian $\Rightarrow$ discrete, real eigenfrequencies ω_n

$$\Rightarrow \quad DOS(\omega) = \sum_n \delta(\omega - \omega_n) \qquad \text{(one "spike" per mode)}$$

$$\Longleftrightarrow \quad \int_{\omega_a}^{\omega_b} DOS(\omega)\, d\omega = \#\text{ eigenvalues in } [\omega_a, \omega_b]$$

Next step up: supercell of P unit cells of size a (in 1d)



with periodic boundaries ($x \Leftrightarrow x + Pa$)

if Bloch modes of ∞ periodic system are $H_k(x) e^{ikx}$,

eigenfunctions of P-periodic system are $H_k e^{ikx}$ for $e^{ik(Pa)} = 1$

$\Longleftrightarrow k = \frac{2\pi}{Pa} p$ for $p = 0, 1, \ldots P-1$

(note: $p + P \Rightarrow k + \frac{2\pi}{a}$ = same sol as k)

$\Rightarrow$ per-period DOS $= DOS(\omega) / P$

$$= \frac{1}{\cancel{P}} \sum_{p=0}^{P-1} \sum_n \delta\left(\omega - \omega_n\left(\tfrac{2\pi p}{Pa}\right)\right) \cdot \underbrace{\frac{2\pi}{Pa}}_{\Delta k} \cdot \frac{\cancel{P} a}{2\pi} \xrightarrow{P \to \infty} \boxed{\frac{a}{2\pi} \int_0^{2\pi/a} dk \sum_n \delta(\omega - \omega_n(k))}$$

* 1d Van Hove example ... (see other handout)
* even better: insted of per - period DOS,

define a per - point DOS = $LDOS(\vec{x}, \omega)$

or even a per - point, per - polarization(j) $LDOS_j^{\omega}(\vec{x})$

such that $DOS(\omega) = \sum_j \int dx \; LDOS_j^{\omega}(\vec{x})$

... see other handout ...
(last page)

Local density of states

suppose we have current $\vec{J} = \hat{e}_j \, \delta(\vec{x}-\vec{x}_0) \, e^{-i\omega t}$

(pt. dipole)

local density of states (LDOS) $\sim$

P = radiated/dissipated power

$$= -\left(\text{power exerted on } \vec{J} \text{ by } \vec{E}\right) = -\tfrac{1}{2}\int d^3x \; \mathrm{Re}\,[E^* \cdot J]$$

$$= -\tfrac{1}{2}\mathrm{Re}\left[E_j^*(\vec{x}_0)\right]$$, where $\vec{E}$ is field produced by $\vec{J}$

$$\left[\nabla\times\nabla\times - \frac{\omega^2}{c^2}\varepsilon\right]\vec{E} = i\omega\mu_0\vec{J}$$

$$\Rightarrow P = -\frac{1}{2}\,\mathrm{Re}\left[\frac{1}{\nabla\times\nabla\times - \frac{\omega^2}{c^2}\varepsilon}\, i\omega\mu_0\delta(x-x_0)\,\hat{e}_j\right]_j(\vec{x}_0)$$

dyadic Green's function : $\left[\nabla\times\nabla\times - \frac{\omega^2}{c^2}\varepsilon\right]\vec{G}^\omega_j(\vec{x},\vec{x}\,') = \delta(\vec{x}-\vec{x}\,')\,\hat{e}_j$

$$\Rightarrow G^\omega_{ij}(\vec{x},\vec{x}\,')$$

$$\Rightarrow P = -\frac{1}{2}\,\mathrm{Re}\left[i\omega\mu_0\, G^{\omega_0}_{jj}(\vec{x}_0,\vec{x}_0)\right]$$

$$= \frac{\omega\mu_0}{2}\,\mathrm{Im}\left[G^\omega_{jj}(\vec{x}_0,\vec{x}_0)\right] \sim \mathrm{LDOS}^{\omega_0}_j(x_0)$$

imag. part of diagonal of Green's function

relate to eigenmodes ...

$$G^{\omega}_{ij}(x,x') = \left(\frac{1}{\nabla\times\nabla\times - \frac{\omega^2}{c^2}\varepsilon}\, \hat{e}_j\, \delta(x-x')\right)\Bigg|_{i,x}$$

assume a complete orthonormal basis $\int \varepsilon \vec{E}^{n*} \cdot \vec{E}^m = \delta_{nm}$

of eigenfunctions $\vec{E}^n(\vec{x})$: $\nabla\times\nabla\times E_n = \frac{\omega_n^2}{c^2}\varepsilon \vec{E}_n$

$$\Rightarrow \hat{e}_j\, \delta(x-x') = \sum_n \vec{E}^n(x) \int \varepsilon \vec{E}^n(x'')^* \cdot \hat{e}_j \delta(x''-x')\, d^3x''$$

$$= \sum_n \varepsilon(x') E^n_j(x')^* \vec{E}^n(x)$$

$$\Rightarrow G^{\omega}_{ij} = \frac{1}{\nabla\times\nabla\times - \frac{\omega^2}{c^2}\varepsilon} \sum_n \varepsilon(x') E^n_j(x')^* \vec{E}^n(x) \Bigg|_{i,x}$$

$$= \sum_n \frac{\varepsilon(x') E^n_j(x')^* E^n_i(x)}{(\omega_n^2 - \omega^2)\frac{\varepsilon(x)}{c^2}}$$

$$\underset{\text{"}}{} (\omega_n+\omega)(\omega_n-\omega)$$

boundary condition : $E \to 0$ at ∞, no incoming waves from ∞

$\Leftrightarrow$ add infinitesimal dissipation $\varepsilon \to \varepsilon + i0^+$

$\omega_n \to \omega_n - i0^+$

distribution theory or complex analy. : $\frac{1}{\omega_n - \omega + i0^+} = \Pr\left[\frac{1}{\omega_n-\omega}\right] + i\pi\delta(\omega-\omega_n)$

$$\Rightarrow LDOS^{\omega}_j(\vec{x}_0) \simeq \sum_n |\vec{E}_j(x_0)|^2\, \delta(\omega-\omega_n) \cdot \frac{\mu_0}{4}$$

= "density" of eigenmodes in j'th direction at x_0 for frequency ω

density of states $DOS(\omega)$

$$= \sum_j \int d^3x \; LDOS_j^\omega(\vec{x}) \;=\; \sum_n \delta(\omega-\omega_n)$$

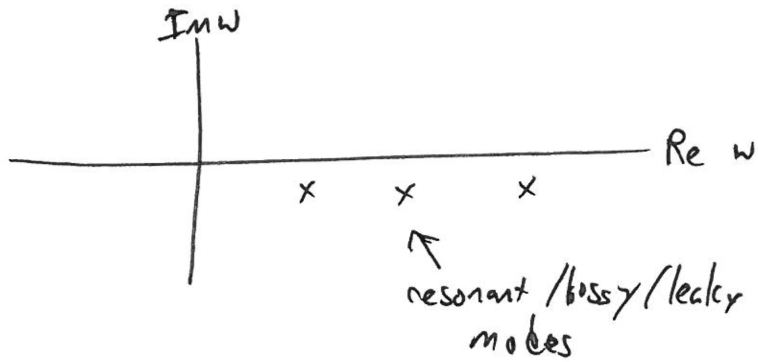
$$\Rightarrow \; LDOS_j^\omega(\vec{x}) = \sum_n \varepsilon |E_j(x_0)|^2 \, \delta(\omega-\omega_n)$$

& $DOS(\omega) \sim \mathrm{Im}\,[\,\underbrace{\text{trace}}_{\text{sum over } j,\, x_0}\; G^\omega\,]$

* a leaky mode / resonant mode:

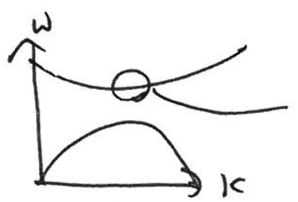
– "complex" frequency ω_0 ($\mathrm{Im}\,\omega_0 < 0$)

really pole in G below real-ω axis



$\Rightarrow$ LDOS in cavity

* Van Hove singularity: 1d example



band edge $\omega \approx \omega_0 + \alpha\left(k - \frac{\pi}{a}\right)^2$

$$DOS(\omega) \approx \int dk \; \delta\left(\omega - \omega_0 - \alpha\left(k-\frac{\pi}{a}\right)^2\right)$$

$$= \int dk \; \frac{\delta\left(k - \frac{\pi}{a} \pm \sqrt{\frac{\omega-\omega_0}{\alpha}}\right)}{2\alpha\,(k-\pi/a)} \sim \frac{1}{\sqrt{\omega-\omega_0}}$$

$\left(k-\frac{\pi}{a}\right)^2 = \frac{\omega-\omega_0}{\alpha}$

$k = \frac{\pi}{a} \pm \sqrt{\frac{\omega-\omega_0}{\alpha}}$