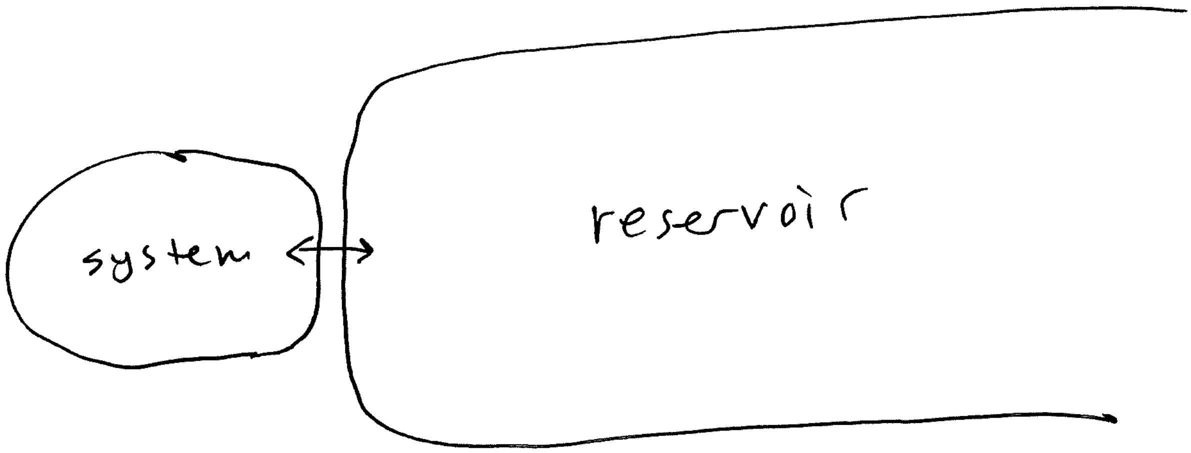
Lec. 12

Energy - time uncertainty

Open quantum system



$$\hat{H} = \hat{H}_{sys} + \hat{H}_{res} + \hat{H}_{int}$$

$$\hat{H}_{sys} = \sum_{n,m} H_{nm} |n\rangle\langle m|$$

$$\hat{H}_{res} = \sum_{k} \varepsilon_k |k\rangle\langle k|$$

$$\hat{H}_{int} = \sum_{n,k} \left(V_{nk} |n\rangle\langle k| + H.c. \right)$$

Retarded Green's function

Let $\quad G^r(t) = -\dfrac{i\,\theta(t)}{\hbar} \hat{U}(t)$

$$\hat{U}(t) = \exp\left(-i \frac{\hat{H} t}{\hbar}\right)$$

$$i\hbar \frac{d}{dt} G^r(t) = \delta(t) + \hat{H} G^r(t)$$

$$\left(i\hbar \frac{d}{dt} - \hat{H}\right) G^r(t) = \delta(t)$$

suppose we are only interested in/ able to measure the observables in the small quantum system, not the large reservoir weakly coupled to it.

These can be obtained from the submatrix of $G^r(t)$:

$$G^r_{nm}(t) = -i \frac{\theta(t)}{\hbar} \langle n | \hat{U}(t) | m \rangle ,$$

where $|n\rangle, |m\rangle \in \mathcal{H}_{sys}$ = system Hilbert space.

$$i\hbar \frac{d}{dt} G^r_{nm}(t) = \delta(t) \langle n|m\rangle - i \frac{\theta(t)}{\hbar} \langle n | \hat{H} \hat{U}(t) | m \rangle$$

Fourier transform of $G^r(t)$

$$G^r(\omega) = \int_{-\infty}^{\infty} dt\; e^{i\omega t}\, G^r(t)$$

$$(\hbar\omega - \hat{H})\, G^r(\omega) = \mathbb{1}$$

$$G^r(\omega) = (\hbar\omega - \hat{H} + i0^+)^{-1}$$

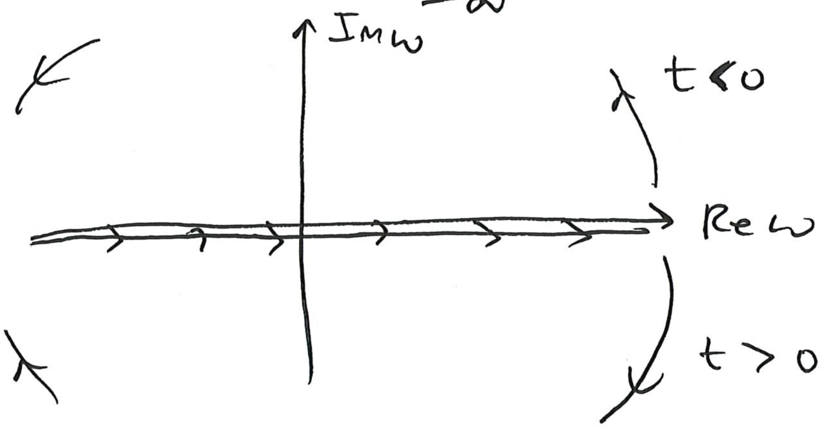
needed for causality

Let $\hat{H}|\nu\rangle = E_\nu |\nu\rangle$

$$G^r(\omega) = \sum_\nu \frac{|\nu\rangle\langle\nu|}{\hbar\omega - E_\nu + i0^+}$$

$$G^r(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, G^r(\omega) = -\frac{i\theta(t)}{\hbar} \sum_\nu e^{-\frac{iE_\nu t}{\hbar}} |\nu\rangle\langle\nu|$$

$$= -\frac{i\theta(t)}{\hbar}\, \hat{U}(t)$$



Spectral function

$$A(\omega) = \frac{i}{2\pi}\left[G^r(\omega) - G^a(\omega)\right]$$

$$= \sum_\nu |\nu\rangle\langle\nu| \, \delta(\hbar\omega - E_\nu)$$

density of states

$$g(\omega) = \mathrm{Tr}\{A(\omega)\} = \sum_\nu \delta(\hbar\omega - E_\nu)$$

→ spectrum of system

Here we have used the identity

$$\lim_{\eta\to 0^+} \frac{1}{x+i\eta} = \mathcal{P}\frac{1}{x} - i\pi\,\delta(x)$$

(see books on Complex variable theory.)

$$G^a(\omega) = \left[G^r(\omega)\right]^\dagger$$

$$i\hbar \frac{d}{dt} G^r_{nm}(t) = \delta(t)\,\delta_{nm} - \frac{i\theta(t)}{\hbar}\left(\sum_{n'} \langle n|\hat{H}|n'\rangle\langle n'|\hat{U}(t)|m\rangle + \sum_{k} \langle n|\hat{H}|k\rangle\langle k|\hat{U}(t)|m\rangle\right)$$

$$i\hbar \frac{d}{dt} G^r_{nm}(t) = \delta(t)\,\delta_{nm} + \sum_{n'} H_{nn'}\, G^r_{n'm}(t) + \sum_{k} V_{nk}\, G^r_{km}(t)$$

$$i\hbar \frac{d}{dt} G^r_{km}(t) = -\frac{i\theta(t)}{\hbar}\langle k|\hat{H}\,\hat{U}(t)|m\rangle$$

$$= -\frac{i\theta(t)}{\hbar}\left(\sum_{k'} \langle k|\hat{H}|k'\rangle\langle k'|\hat{U}(t)|m\rangle + \sum_{n'} \langle k|\hat{H}|n'\rangle\langle n'|\hat{U}(t)|m\rangle\right)$$

$$i\hbar \frac{d}{dt} G^r_{km}(t) = \varepsilon_k\, G^r_{km}(t) + \sum_{n'} V_{kn'}\, G^r_{n'm}(t)$$

Fourier transform

$$\left(\hbar\omega - \varepsilon_k + i0^+\right) G^r_{km}(\omega) = \sum_{n'} V_{kn'} G^r_{n'm}(\omega)$$

causality

$$G^r_{km}(\omega) = \frac{1}{\hbar\omega - \varepsilon_k + i0^+} \sum_{n'} V_{kn'} G^r_{n'm}(\omega)$$

$$\sum_{n'} \left(\hbar\omega\,\delta_{nn'} - H_{nn'} + i0^+\right) G^r_{n'm}(\omega) = \delta_{nm} + \sum_k V_{nk} G^r_{km}(\omega)$$

$$= \delta_{nm} + \sum_{k,n'} \frac{V_{nk} V_{kn'}}{\hbar\omega - \varepsilon_k + i0^+} G^r_{n'm}(\omega)$$

Let $\Sigma^r_{nn'}(\omega) \equiv \sum_k \frac{V_{nk} V_{kn'}}{\hbar\omega - \varepsilon_k + i0^+}$

$$\left(\mathbb{1}\hbar\omega - \hat{H}_{sys} - \hat{\Sigma}^r(\omega)\right) G^r_{sys}(\omega) = \mathbb{1}$$

$$G^r_{sys}(\omega) = \left(\mathbb{1}\hbar\omega - \hat{H}_{sys} - \hat{\Sigma}^r(\omega)\right)^{-1}$$

$$\Sigma^r(\omega) = \sigma(\omega) - \frac{i}{2}\Gamma(\omega),$$

where

$$\sigma_{nm}(\omega) = \mathcal{P} \sum_k \frac{V_{nk} V_{km}}{\hbar\omega - \varepsilon_k}$$

$$\Gamma_{nm}(\omega) = 2\pi \sum_k V_{nk} V_{km} \, \delta(\hbar\omega - \varepsilon_k)$$

$$= 2\pi \, \overline{V_{nk} V_{km}} \; \underbrace{g_{res}(\hbar\omega)}_{\text{density of states of reservoir}}$$

cf. Fermi's golden rule

$\sigma(\omega)$ simply shifts the system energy levels, but $\Gamma(\omega)$ moves the energy values off the real axis, leading to broadening, and is qualitatively more significant.

<u>Simple case</u> $\quad \sigma(\omega) = 0$

$$\Gamma(\omega) = \Gamma \, \mathbb{1}$$

$$G^r_{sys}(\omega) = \left(\mathbb{1}\hbar\omega - \hat{H}_{sys} + i\Gamma/2\right)^{-1}$$

Let $\hat{H}_{sys}|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle$.

$$G^r_{sys}(\omega) = \sum_\alpha \frac{|\alpha\rangle\langle\alpha|}{\hbar\omega - \varepsilon_\alpha + i\Gamma/2}$$

$$A_{sys}(\omega) = \frac{i}{2\pi}\left[G^r_{sys}(\omega) - G^a_{sys}(\omega)\right]$$

$$= \frac{i}{2\pi}\sum_\alpha |\alpha\rangle\langle\alpha| \left(\frac{1}{\hbar\omega - \varepsilon_\alpha + i\Gamma/2} - \frac{1}{\hbar\omega - \varepsilon_\alpha - i\Gamma/2}\right)$$

$$= \sum_\alpha \frac{|\alpha\rangle\langle\alpha|\,\Gamma/2\pi}{(\hbar\omega - E_\alpha)^2 + (\Gamma/2)^2}$$

$$g_{sys}(\omega) = \mathrm{Tr}\{A_{sys}(\omega)\} = \mathrm{Tr}_{sys}\{A(\omega)\}$$

$$= \sum_\alpha \frac{\Gamma/2\pi}{(\hbar\omega - \varepsilon_\alpha)^2 + (\Gamma/2)^2}$$

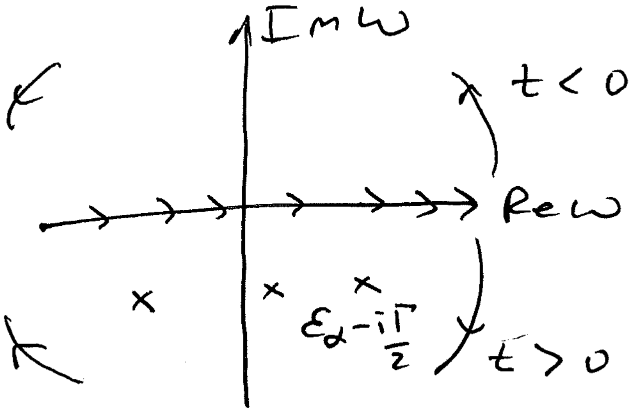
Energy levels broadened into Lorentzians,

FWHM $= \Gamma$.

Let's Fourier transform back to the time domain:

$$G^r(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, G^r(\omega)\, e^{-i\omega t}$$

$$= \sum_\alpha |\alpha\rangle\langle\alpha| \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \frac{e^{-i\omega t}}{\hbar\omega - \varepsilon_\alpha + i\Gamma/2}$$



$$= -\frac{i\theta(t)}{\hbar} \sum_\alpha |\alpha\rangle\langle\alpha| \times e^{-i\frac{\varepsilon_\alpha t}{\hbar} - \frac{\Gamma t}{2\hbar}}$$

$$|G^r_{\alpha\alpha}(t)|^2 = \frac{1}{\hbar^2}\theta(t)\, e^{-\frac{\Gamma t}{\hbar}}$$

$$\equiv \frac{\theta(t)}{\hbar^2}\, e^{-t/\tau}$$

$$\boxed{\begin{aligned} &\text{lifetime} \quad \tau = \frac{\hbar}{\Gamma} \equiv \Delta t \\ &\Delta E = \frac{\Gamma}{2} = \text{HWHM} \\ &\Delta E\, \Delta t = \frac{\Gamma}{2}\frac{\hbar}{\Gamma} = \frac{\hbar}{2} \qquad \text{Energy-time uncertainty relation} \end{aligned}}$$