

Quantum Transport:

ATOM TO TRANSISTOR

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Lecture 29: Level Broadening: Irreversibility

Ref. Chapter 8.4



Network for Computational Nanotechnology

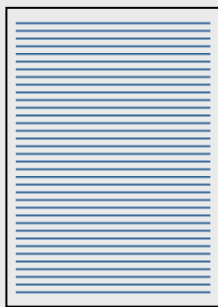
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Device and Reservoir

- Continued from last time, we were looking at a device coupled to a reservoir by $[\tau]$.

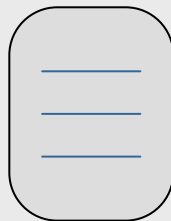
Device Coupled to a Reservoir

reservoir $[\tau]$



$[H_R]$

device



$[H]$

- The system Hamiltonian and Green's function are

$$\bar{H} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R \end{bmatrix}$$

and

$$\bar{G} = [E\bar{I} - \bar{H} + i0^+]^{-1} = \begin{bmatrix} G & G_{Rd} \\ G_{dR} & G_R \end{bmatrix}$$

where the device part of Green's function, G , is defined as

$$G = [EI - H - \Sigma]^{-1}$$

with self energy $\Sigma = \tau g_R \tau^+$

and surface Green's function g_R

- From the Green's function we can derive the spectral function

$$A(E) = i(G - G^+)$$

which provides the LDOS along its diagonal

- Why do we want the local density of states? *Answer: It provides a very important meeting ground for theory and experiment.* Using scanning probe microscopy one can physically measure the LDOS on an atomic scale.

- Physically, the Green's function is best interpreted in the time domain

$$G(t) = e^{-i\varepsilon t/\hbar} e^{-i\Sigma t/\hbar} \theta(t)$$

Where the effect of Σ is to add to the energy level and broaden the wave function such that

$$G(t) = e^{-i\varepsilon' t/\hbar} e^{-\gamma t/2\hbar}$$

$$\varepsilon' = \varepsilon + \text{Re} \{ \Sigma \}$$

$$\gamma = -2 \text{Im} \{ \Sigma \}$$

(ignore for now the fact that Σ is also energy dependent)

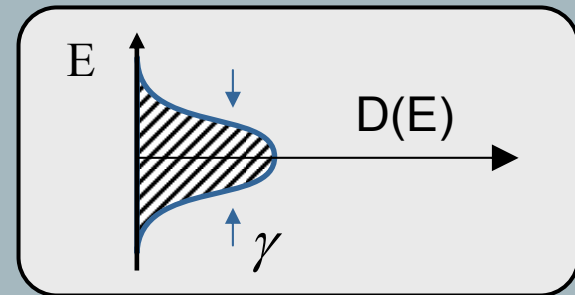
- The relation between broadening, the Green's function, and self-energy is best illustrated by looking at a 1-level device. In the energy domain a 1-level device has

$$G = \frac{1}{E - \varepsilon' + i\gamma/2}$$

such that

$$\begin{aligned} A &= i(G - G^+) = \frac{\gamma}{(E - \varepsilon')^2 + (\gamma/2)^2} \\ &= 2\pi(LDOS) = 2\pi(DOS) \end{aligned}$$

- Plotting the local density of states we see



which is the well known Lorentzian of a broadened level!

Side note: There is an inverse relationship between broadening, γ , and lifetime, τ

$$\gamma \times \tau = \hbar$$

Infinitesimal Term

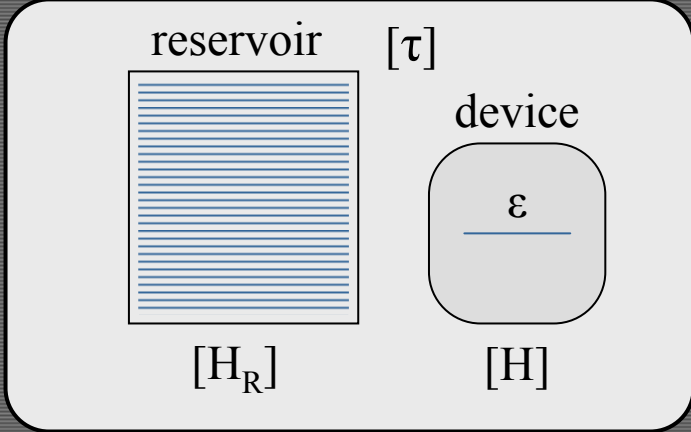
- Now consider $+i0$ in the Green's function definition

$$G = [EI - H + i0^+]^{-1}$$

It is because of the introduced $i0^+$ that Σ is non-Hermitian; mathematically one could argue that this has to be added to make the Fourier transform converge, how ever how would we justify the presence of this infinitesimal term which has profound physical implications?

- To gain a better understanding, let us look at a 1-level device and a reservoir.

Device decoupled from a Reservoir

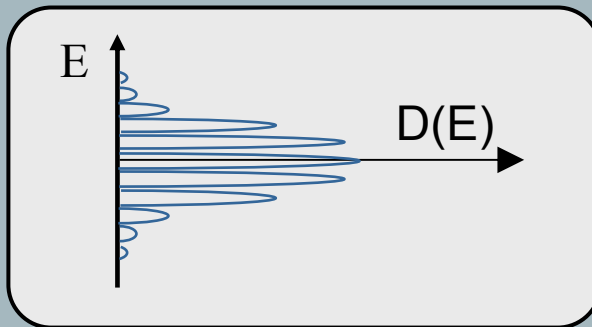


- In the eigenstate basis with the device and reservoir decoupled the spectral function is
- $$\frac{A(E)}{2\pi} = \begin{bmatrix} \delta(E - \epsilon) & & & & \\ & \delta(E - \epsilon_0) & & & \\ & & \delta(E - \epsilon_1) & & \\ & & & \ddots & \\ & & & & \dots \end{bmatrix}$$

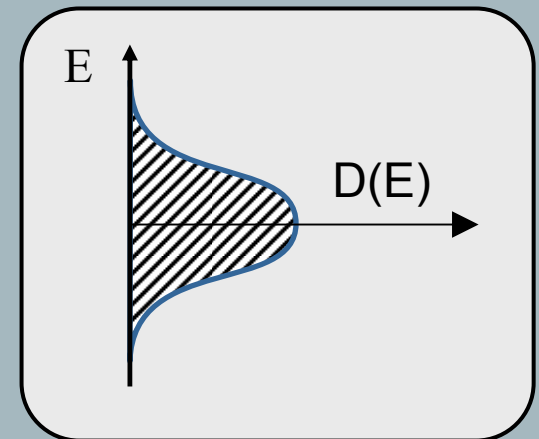
- Similarly, when coupled together the system Hamiltonian becomes

$$\bar{H} = \begin{bmatrix} \varepsilon & \tau_1 & \tau_2 & \dots \\ \tau_1^+ & \varepsilon_1 & & \\ \tau_2^+ & & \varepsilon_2 & \\ \vdots & & & \ddots \end{bmatrix}$$

- Mixing occurs, with wavefunctions leaking from both sides, and the resulting LDOS on the device looks like...



- Essentially, what the $i0^+$ term does is broaden out these “spikes” into a continuous DOS...

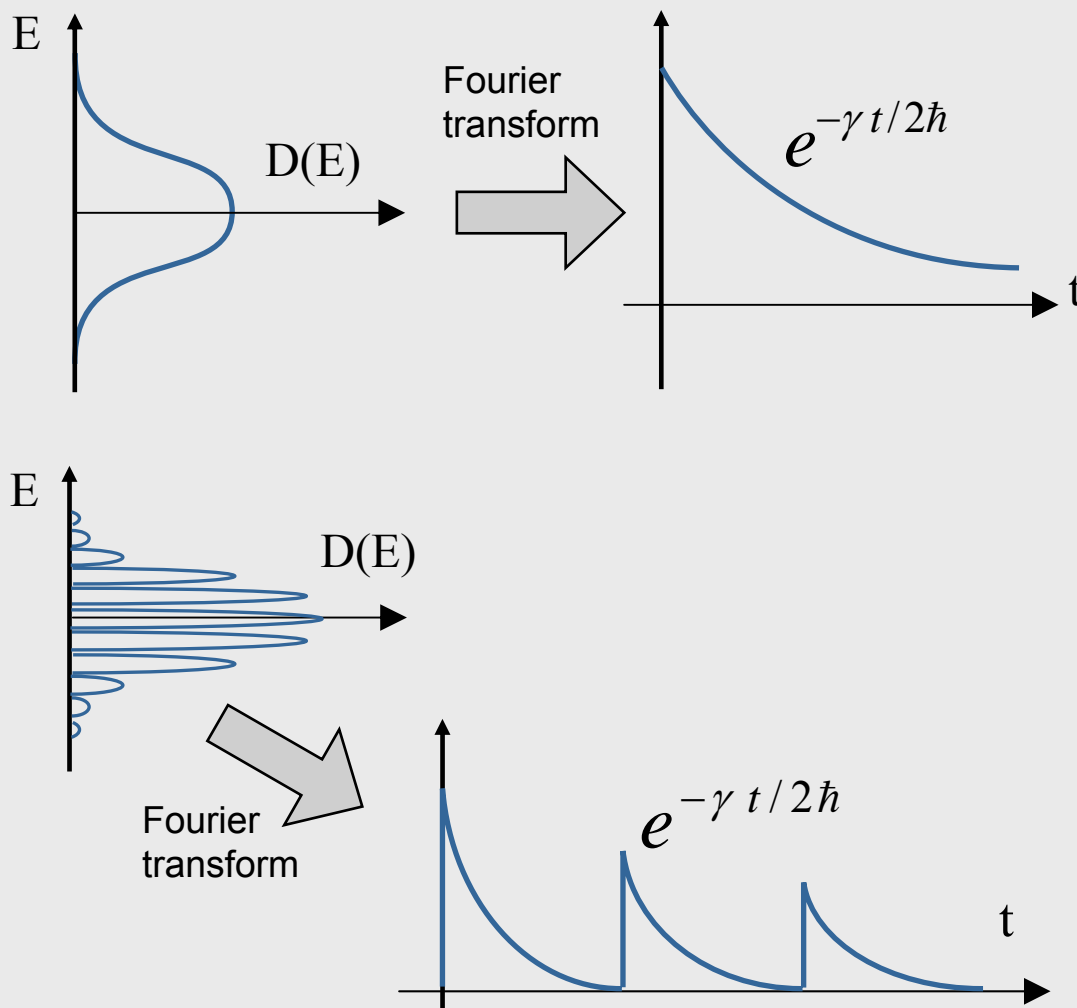


- Important question: What is the physical difference between the system for which the LDOS are spiked compared with a system where the infinitesimal term has broadened out these levels to a smooth distribution states?

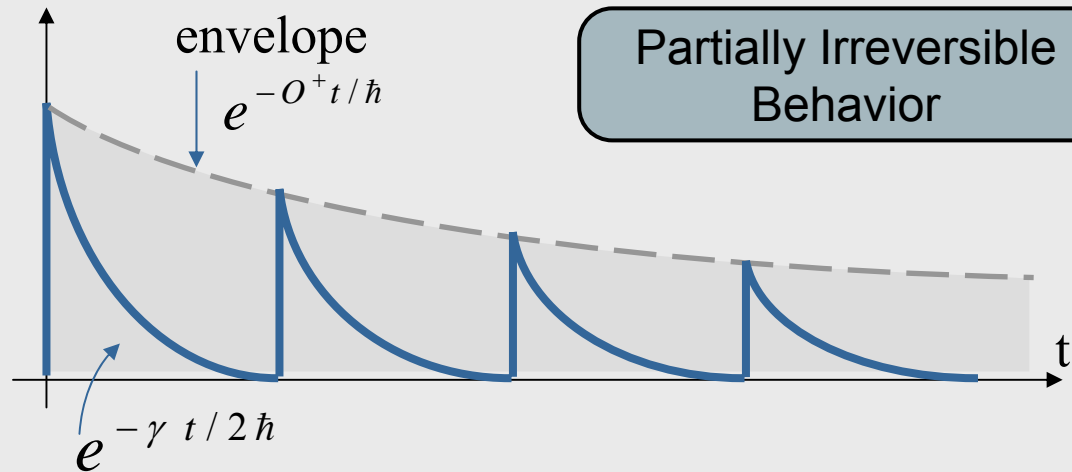
Time Domain Infinitesimal

- The difference in behavior of the system for a continuous or discrete DOS is best illustrated in the time domain.

- Observing these plots we see that the “spiked” DOS represents a reversible repeating system (or an electron oscillating back and forth between the device and reservoir) with repetition time $T = (2\pi\hbar) / (\Delta E)$ whereas the continuous DOS represents a non-reversible DOS.



- In effect, what $i0^+$ does is add an irreversibility decay in the time domain, preventing the electron from oscillating back and forth from the reservoir. This is how it broadens the DOS, it acts as a dampening factor and thereby allows us to model the irreversible physical nature of most infinite systems with finite sized numerical models.



- As a rule of thumb O^+ must be greater than the spacing between energy levels in the reservoir (ΔE). However, often Σ is big enough and ΔE small enough in large reservoirs that broadening of the peaks is already taken care of. Note: the behavior of $e^{-\gamma t/2\hbar}$ is separate from that of $e^{-O^+t/\hbar}$

Interpretation of $\text{Im}(\Sigma)$

- Moving on, recall from last time we defined the self-energy Σ as

$$\Sigma = \tau G_R \tau^+$$

Though G_R is very big, τ is only non-zero at the coupling surface, therefore we have:

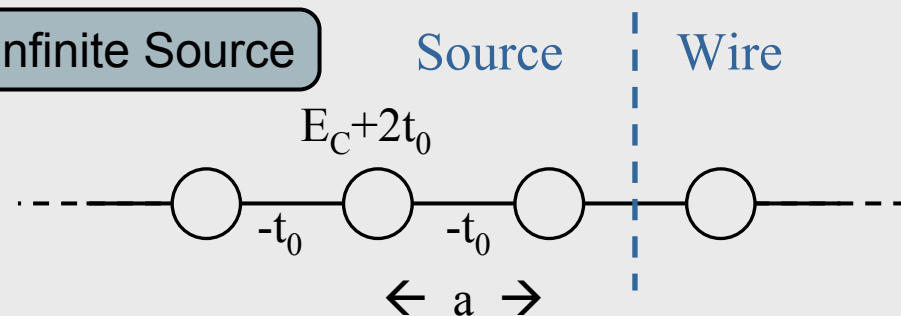
$$\Sigma = \tau g_R \tau^+$$

where g_R is the surface Green's function

- For a 1-D wire coupled to an infinite 1-D source we arrived at

$$\Sigma = t_0 \left(\frac{-e^{ika}}{t_0} \right) t_0 = -t_0 e^{ika}$$

Wire and Infinite Source



- Now looking at the imaginary part of the self energy we get $\gamma = -2 \text{Im}\{\Sigma\}$

$$= +2t_0 \sin ka$$

Interpretation of $\text{Im}(\Sigma)$

- The E-k relationship for a 1-D wire is

$$E = E_C + 2t_0(1 - \cos ka)$$

with the state velocity given as

$$v = \frac{1}{\hbar} \frac{dE}{dk} = \frac{2at_0 \sin ka}{\hbar}$$

Leading to the observation

$$\gamma = \frac{\hbar v}{a}$$

and so the lifetime of an electron at the coupling surface is

$$\frac{1}{\tau} = \frac{\gamma}{\hbar} = \frac{v}{a}$$

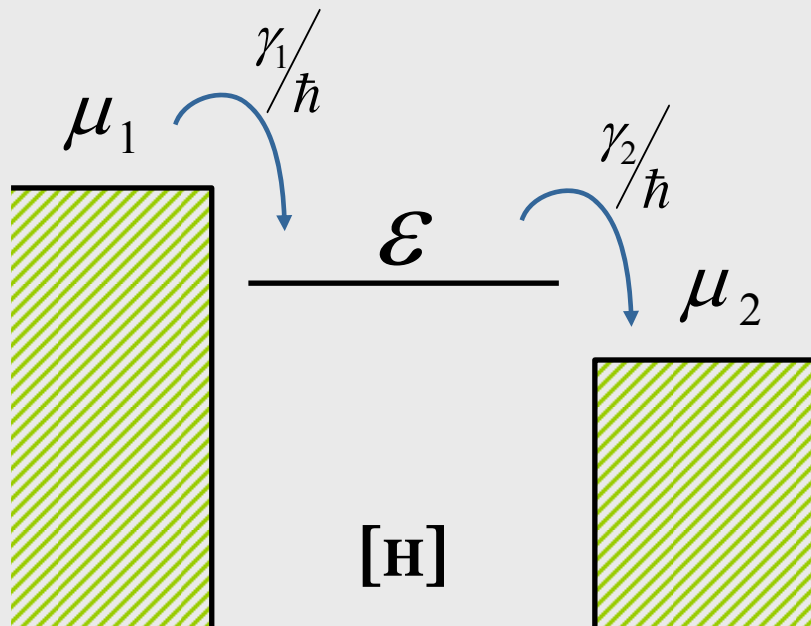
- This provides a relation between self-energy and the velocity at which an electron escapes from a reservoir coupling unit cell into the device

- Final Comment:

In future lectures we will concentrate on reservoirs that can be modeled by a 1-D wire, but it is important to note that self-energy, Σ , is a general concept which may be applied to any 2-D or 3-D geometry

- In the next few lectures we will return to the problem of current flow

Current Flow Through a 1-Level Device



- Where current is given by

$$I = \frac{2q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2)$$

or more exactly (considering broadening as the result of strong coupling) as

$$I = \frac{2q}{\hbar} \int dE \bar{T}(E) (f_1 - f_2)$$

$\bar{T}(E)$ is known as the transmission function, it is proportional to the DOS and $\frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}$

- In matrix from the imaginary part of Σ can be written as $\Gamma = i(\Sigma - \Sigma^+)$

- More precise non-equilibrium calculations demand that γ_1 and γ_2 are no longer constants but follow from $\Sigma_{1,2}$ such that

$$\begin{aligned}\Sigma_{1,2} &= \frac{\Sigma_{1,2} + \Sigma_{1,2}^+}{2} + \frac{\Sigma_{1,2} - \Sigma_{1,2}^+}{2} \\ &= \frac{\Sigma_{1,2} + \Sigma_{1,2}^+}{2} - \frac{i\Gamma_{1,2}}{2}\end{aligned}$$

where $\Gamma_{1,2}$ is responsible for broadening and is energy dependent

- The transmission $\bar{T}(E)$, can be calculated from a knowledge of $[H]$, $[\Sigma_1]$ and $[\Sigma_2]$

- We'll discuss transmission more in depth in the next few lectures.