Quantum Transport:
Atom to Transistor

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Lecture 26: Level Broadening: Open Systems and LDOS
Ref. Chapter 8.1 & 8.2
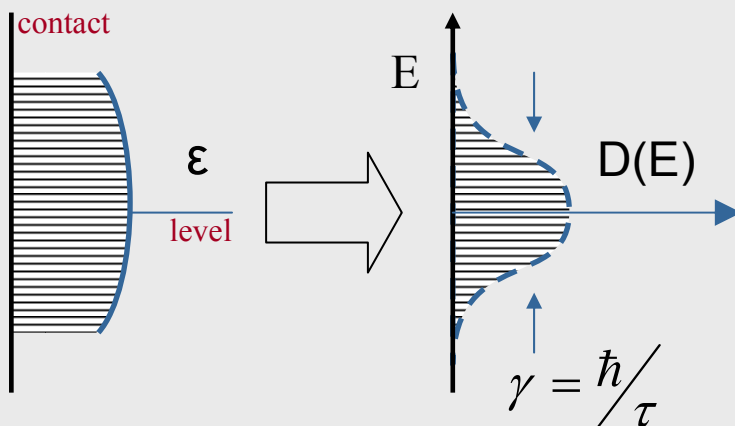
Network for Computational Nanotechnology

• As stated in early lectures, the coupling of a device to contact reservoir leads to what is known as level broadening

Single Level Broadening

• Let us start with a very important concept: "local density of states" (LDOS)

• Recall, for a closed or equilibrium system from the Hamiltonian, [H], one can easily find the density matrix, and electron density (diagonal elements of density matrix in real space representation), via

$$[\rho] = f_0([H] - \mu[I])$$

But for open systems the relation is not so simple i.e. a device that is in contact with a very large contact.

• The width of DOS depends on the strength of coupling to the contact. Weak coupling will collapse DOS to a delta function (0 broadening) while stronger coupling results in a more broadened DOS.


$$\gamma = \hbar / \tau$$

• One way to justify broadening is that for an isolated system, the electron and so as the electron wave function will stay in the level for ever. How ever for a system in contact, the electron will escape into to the reservoir. Or in other words the wave function in the system has a decay time. Mathematically speaking the wave function changes from $e^{-iEt/\hbar}$ for an isolated system to $e^{-iEt/\hbar}e^{-t/\tau}$ for a system in contact. Looking at DOS as the Fourier transform of the wave function, it will be a delta function without a lifetime and it will look broadened when the electron has a finite lifetime. Stronger coupling → Shorter Lifetime → Bigger broadening. Today we want to understand broadening without using the concept of lifetime.
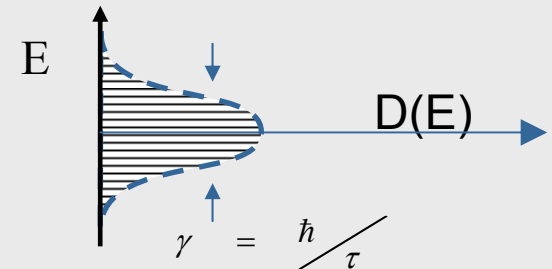
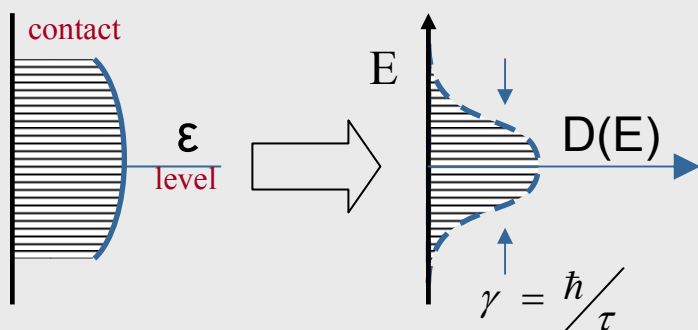• Looking at the density of states for an isolated single level…

$$\varepsilon$$
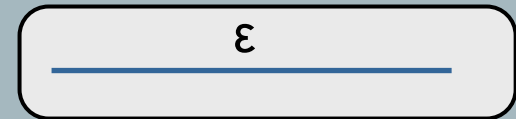
… and reservoir
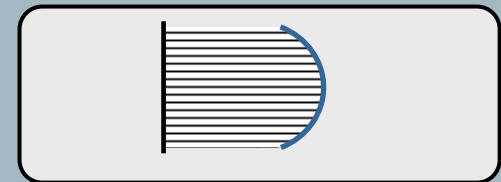
… we could write total DOS for the whole system:

$$DOS(E) = \delta(E - \varepsilon) + \sum_R \delta(E - \varepsilon_R)$$

• When these two elements are brought together as…

contact

E

ε level
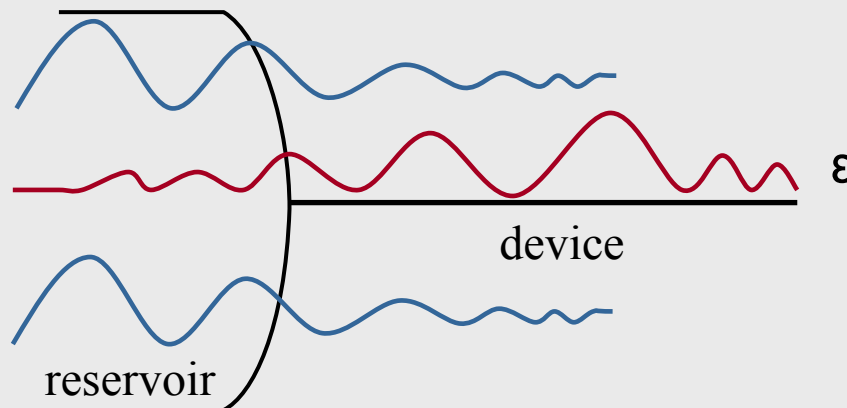
D(E)

$\gamma = \hbar/\tau$

…the observed broadening may be explained by considering the "**local density of states**" in the device. Which is

$$\sum_{\alpha}\left|\phi_{\alpha}(d)\right|^{2}\delta(E-\varepsilon_{\alpha})$$

where "d" is the device

• Upon coupling, reservoir wave functions do not lie only in the reservoir but also "leak" into the device. Similarly, the device wavefunction will "leak" slightly into the reservoir

Wavefunction Leakage

ε

device

reservoir

• Notice that when the channel is coupled to the reservoir, the single level previously described as a delta function (which can hold one electron) broadens into a distribution of states SUM of which can contain ONLY one electron. What happens is that the level looses a part of wave function to the contact at a certain energy and gains some at another energy. What is true and not obvious is that what it looses is equal to what it gains so at the end the overall broadened levels can still contain only one electron. (not considering spin)

• In order to understand broadening, one needs to look at the Local Density of States. (LDOS)

• In general for any simple device the local density of states is expressed as

$$D(\vec{r};E) = \sum_{\alpha} |\phi_{\alpha}(\vec{r})|^2 \delta(E - \varepsilon_{\alpha})$$

This may be viewed more generally as the diagonal elements of the spectral function A (divided by 2π; this is just a convention)

$$A(\vec{r},\vec{r}';E) = 2\pi \sum_{\alpha} \phi_{\alpha}(\vec{r}) \delta(E - \varepsilon_{\alpha}) \phi_{\alpha}^{*}(\vec{r}')$$

• $D(\vec{r}; E)$ shares the same relation to $A(\vec{r}, \vec{r}'; E)$ as the electron density, $n(\vec{r})$, does to the density function $\rho(\vec{r}, \vec{r}')$. Recall,

$$n(\vec{r}) = \sum_\alpha \left| \phi_\alpha(\vec{r}) \right|^2 f_0(\varepsilon_\alpha - \mu)$$

and

$$\rho(\vec{r}, \vec{r}') = \sum_\alpha \phi_\alpha(\vec{r}) f_0(\varepsilon_\alpha - \mu) \phi_\alpha^*(\vec{r}')$$

• As well, if we sum $D(\vec{r}; E)$ across all space we get the density of states and if we sum $n(\vec{r})$ across all space we get the number of electrons (N).

• Similarly, a general matrix notation for the density function
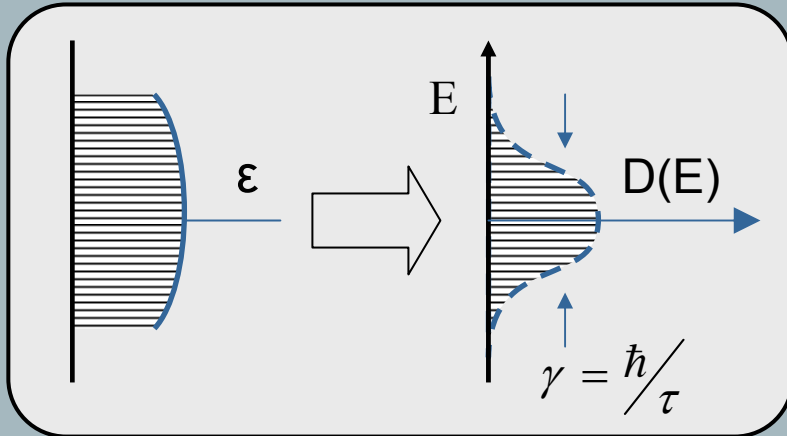
$$[\rho] = f_0([H] - \mu[I])$$

leads to a general matrix formulation for the Spectral Function:

$$[A(E)] = 2\pi\delta(E[I] - [H])$$

• Summary: The spectral function provides the LDOS in any basis

• Now we will prove that, even after broadening, the total number of electrons a level holds is 1

$$\varepsilon \Rightarrow \quad E \quad D(E)$$

$$\gamma = \hbar / \tau$$

• That is, we must prove

$$\int_{-\infty}^{\infty} dE \ D(\bar{r}; E) = 1$$

• But this is the same as the diagonal elements of

$$\int_{-\infty}^{\infty} dE \frac{A(\vec{r}, \vec{r}'; E)}{2\pi}$$

but in the eigenstate basis this is

$$\int_{-\infty}^{\infty} \frac{dE}{2\pi} A(E) = \begin{bmatrix} 1 & 0 & 0 & \\ 0 & 1 & 0 & \\ 0 & 0 & 1 & \cdots \\ & \vdots & & \ddots \end{bmatrix} = [I]$$

since $\int_{-\infty}^{\infty} dE \delta(E - \varepsilon) = 1$

This proves the conjecture since [I] remains the same in ANY basis.

• The spectral function, importantly, may be used to rewrite the density matrix in a new way:

$$[\rho] = f_0([H] - \mu[I])$$

$$= \int dE f_0(E - \mu)\delta(E[I] - [H])$$

$$= \int \frac{dE}{2\pi} f_0(E - \mu)[A(E)]$$

• In dealing with a closed system the old expression for density matrix is easier to do compared to this new expression based on spectral function. However, for open systems like our nano-transistor the story is different. We have to take into account the effect of coupling. There, we can get by using the spectral function looking at DOS inside the device AND considering the effect of coupling to the reservoirs.
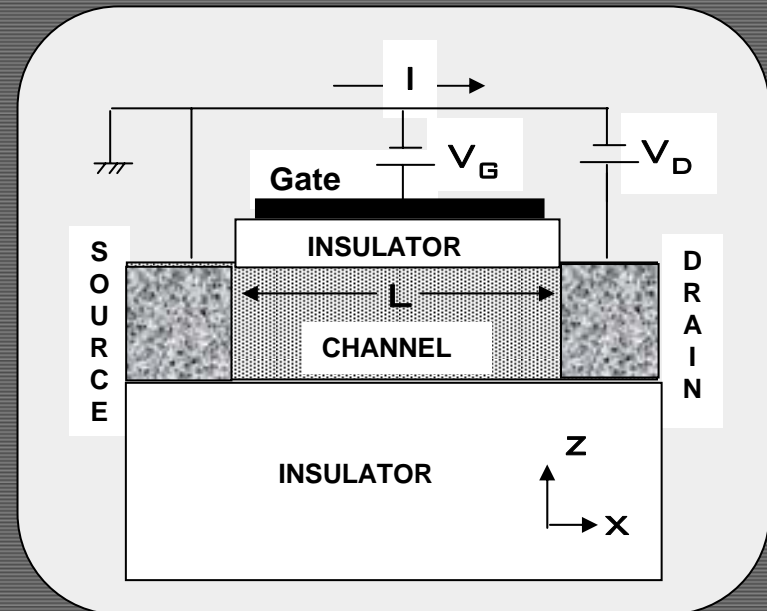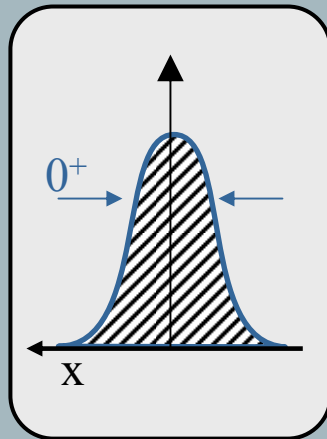

• How is this done? Through the concept of "self-energy" matrices, Σ_1 and Σ_2, which require discussion of Green's functions a concept that is closely related to the spectral function.

• We can represent the delta function, with infinite height and area of 1, as

$$2\pi\delta(x) = \left[\frac{1}{x+i0^+} - \frac{1}{x-i0^+}\right]i$$

$$= \frac{2 \cdot 0^+}{x^2 + \left(0^+\right)^2}$$

Which looks like

with width determined by 0^+, such that width $\approx 0^+$

• Since the spectral function is given by

$$[A(E)] = 2\pi\delta(EI - H)$$

we may now write it as

$$[A(E)] = i\left\{\begin{array}{l}\left[(E+i0^+)I - H\right]^{-1} - \\ \left[(E-i0^+)I - H\right]^{-1}\end{array}\right\}$$

Where, the Green's function, G, is

$$G = \left[(E+i0^+)I - H\right]^{-1}$$

such that:

$$[A(E)] = i\left[G - G^+\right]$$

• When including the infinite reservoirs the Green's function for the device becomes

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

• Notice that the [H] and [Σ] that appear above are of the size of the channel and not that of reservoirs; i.e. in order to describe the channel, you don't have to take the inverse of a matrix that has a huge Hamiltonian describing the whole system; rather you just take the Green's function describing the channel and deal with that which makes things a lot easier computationally. Notice that [Σ] (*self energy*) gives the effect of coupling to the contacts and is important conceptually. For one thing, its imaginary part gives you the lifetime of the electron in the channel. We'll discuss self energy more in depth in the next lecture.