Quantum Transport:
Atom to Transistor

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Lecture 28: Level Broadening: Lifetime

Ref. Chapter 8.3

Network for Computational Nanotechnology

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online simulations and more

General Concepts

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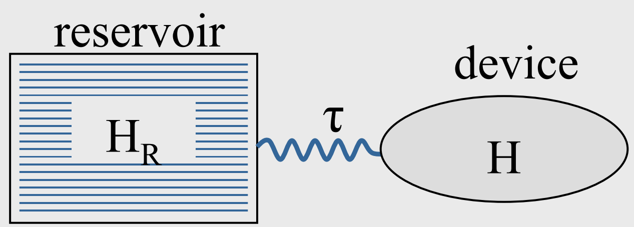
• In this lecture, we will discuss the physical meaning of the Green's function and furthermore the physical interpretation of the self-energy matrix Σ

Device Coupled to a Reservoir



• Continued from last time, we were looking at an open system consisting of a device coupled to a reservoir. The reservoir and device Hamiltonians are H_R and H, with coupling τ between the two.

• Recall, the <u>overall</u> Hamiltonian is $\overline{H} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R \end{bmatrix}$ with a Green's function:

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

and a spectral function:

$$\overline{A} = i(\overline{G} - \overline{G}^+) = 2\pi\delta\left[E\overline{I} - \overline{H}\right]$$

The <u>device</u> Green's function and spectral function are

$$G = \left[EI - H - \Sigma\right]^{-1}$$
$$G^+ = \left[EI - H - \Sigma^+\right]^{-1}$$
$$A = i(G - G^+)$$

• Importantly, the Green's function method allows us to concentrate on the device and not worry about the entire system.

Spectral Function

- Recall, $\Sigma = \tau g_R \tau^+$, where g_R is the surface Green's function. It describes only those points at the reservoir device boundary. And generally we only need to solve the Green's function only for those few points.

- Side Note: A very important property of Σ is that it is anti-Hermitian

- Moving on…
To consider the physical meaning of G(E), we consider the diagonal representation where things are more clear to understand

$$[G(E)] = \begin{bmatrix} \frac{1}{E-\varepsilon_1+i0^+} & 0 & \cdots \\ 0 & \frac{1}{E-\varepsilon_2+i0^+} & \\ \vdots & & \ddots \end{bmatrix}$$

Inverse Fourier Transform

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- Now, let us look at

$$[G(E)] = \begin{bmatrix} \dfrac{1}{E-\varepsilon_1+i0^+} & 0 & \cdots \\ 0 & \dfrac{1}{E-\varepsilon_2+i0^+} & \\ \vdots & & \ddots \end{bmatrix}$$

in the time domain.

- This is done via the Fourier transform $\widetilde{G}(t) = \int \dfrac{dE}{2\pi\hbar} G(E) e^{-iEt/\hbar}$

with inverse transform

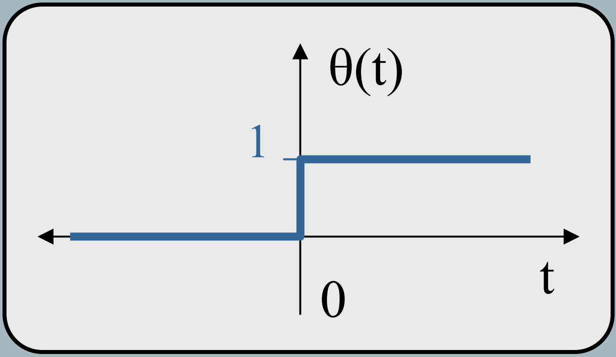
$$G(E) = \int dt G(t) e^{+iEt/\hbar}$$

- Specifically, consider the Fourier transform of one level, say ε_1…

$$\widetilde{G}_{11}(t) = \int \frac{dE}{2\pi\hbar} \left(\frac{1}{E-\varepsilon_1+i0^+} \right) e^{-iEt/\hbar}$$

$$= -\frac{i}{\hbar} \theta(t) e^{-i\varepsilon_1 t/\hbar} e^{-0^+ t}$$

where $\theta(t)$ is the step function



Inverse Fourier Transform

• To see how this works, perform the inverse Fourier transform

$$G_{11}(E) = \int_{-\infty}^{\infty} dt\, \widetilde{G}_{11}(t) e^{+iEt/\hbar}$$

$$= \frac{-i}{\hbar} \int_0^{\infty} dt e^{-i\varepsilon_1 t/\hbar} e^{+iEt/\hbar} e^{-0^+ t}$$

$$= \frac{-i}{\hbar} \left[\frac{e^{i(E-\varepsilon_1)t/\hbar} e^{-0^+ t}}{\left(i(E-\varepsilon_1) - 0^+\right)/\hbar} \right]_0^{\infty}$$

$$= \frac{i}{\hbar} \times \frac{1}{\left(i(E-\varepsilon_1) - 0^+\right)/\hbar}$$

$$= \frac{1}{E - \varepsilon_1 + i0^+}$$

• Thus, $$\widetilde{G}_{11} = \frac{-i}{\hbar} \theta(t) e^{-i\varepsilon_1 t/\hbar} e^{-0^+ t}$$

is the time domain version of the Green's function

• And we can see that it satisfies

$$\left[i\hbar \frac{\partial}{\partial t} - \left(\varepsilon_1 - i0^+\right) \right] \widetilde{G}_{11}(t) = \delta(t)$$

• What does this mean? *Answer: It means that we can physically view the Green's function as the impulse response of the Schrödinger equation*

Impulse Response

- Side note: What is this 0^+ we include with the Green's function? Mathematically we justify it because it makes the Fourier transform converge, but physically it has very subtle meaning

- Main Point: The Green's function, G(t), is the impulse response

$$\left(i\hbar\frac{\partial}{\partial t}-[H]+i0^+[I]\right)G(t)=[I]\delta(t)$$

of the general Schrödinger equation

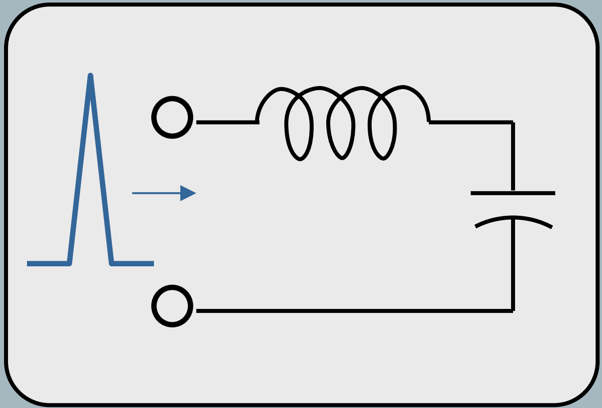
$$\left(i\hbar\frac{\partial}{\partial t}-[H]\right)\{\Psi(t)\}=[0]$$

- In general we can look at the impulse response of any differential equation to get the Green's function for that equation.

e.g. Poisson's Equation

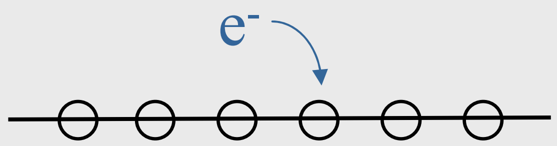
$$\nabla^2\phi=\frac{-\rho}{\varepsilon}\Rightarrow\nabla^2 G=-\delta(\vec{r})$$

or an LC circuit



The Physical Picture

• Example: impulse excitation of the Schrödinger equation in 1-Dimension might be viewed as "injecting" an electron into the well known 1-D wire

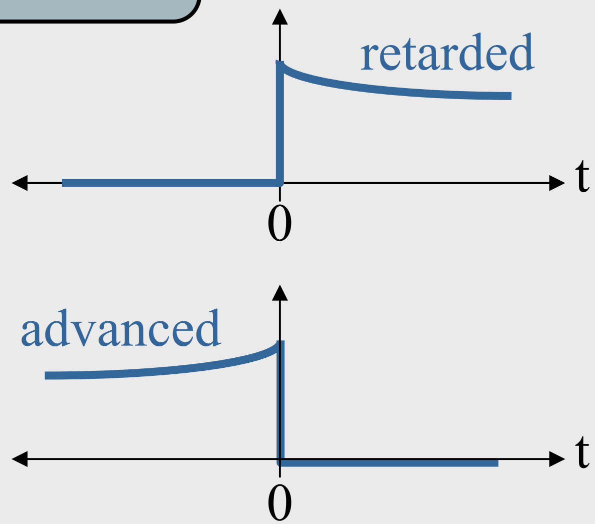


• [G(E)] in the time domain has a range of $0 \leq t < \infty$ and is usually called the "retarded Green's function." $[G(E)]^+$ in the time domain has a range of $-\infty < t \leq 0$ and is usually called the "advanced Green's function"

• Also note that the presence of $+i0^+$ or $-i0^+$ in G and G^+ respectively leads to a world of difference in the time domain. For our simple example G^+ gives

$$G_{11}^{+}(t) = \frac{i}{\hbar}\theta(-t)e^{-i\varepsilon_1 t/\hbar}e^{i0^+ t}$$

Green's Functions



Physical Interpretation of Σ

- We can also apply the concept of "impulse response" to gain insight into the physical meaning of Σ.

- Recall for the device region

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

translated to the time domain this gives…

$$\left(i\hbar\frac{\partial}{\partial t} - H - \Sigma\right)G(t) = I\delta(t)$$

- Let us consider a single level device such that [H] = ε. Therefore we have

$$\left(i\hbar\frac{\partial}{\partial t} - \varepsilon - \Sigma\right)G(t) = \delta(t)$$

Thus,

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

where

$$\varepsilon' = \varepsilon + \mathrm{Re}\left\{\Sigma\right\}$$
$$\gamma = -2\,\mathrm{Im}\left\{\Sigma\right\}$$

Physical Interpretation of Σ

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• Physically the real part of Σ corresponds to an energy level shift in the device. The imaginary part (times –2) represents the rate at which an electron will leak out of the reservoir.

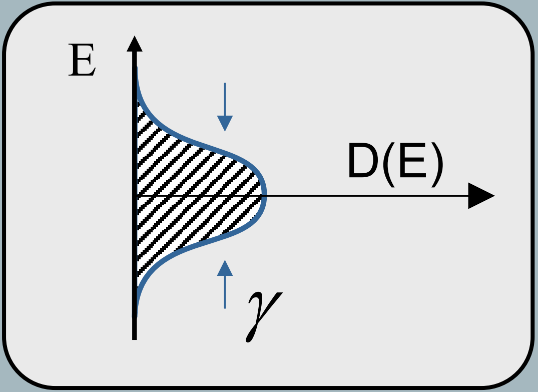
• From $\gamma = -2\,\mathrm{Im}\{\Sigma\}$
we define the lifetime, τ, of an electron state as

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

such that

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

• Also, γ is related to the broadening of a level



such that there exists an “uncertainty” relation between lifetime and broadening

$$\gamma \times t = \hbar$$

Where Broadening Comes From

- How do we know that γ is directly related to the broadening of a level?
- Well, $A(E) = i\left(G - G^{+}\right)$

and for our 1-level device

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

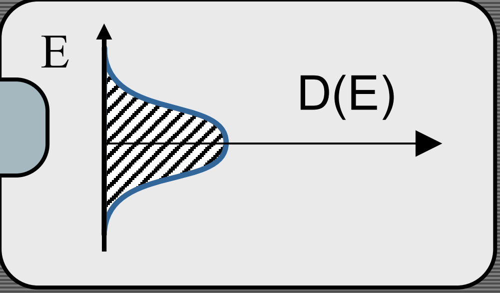
$$\therefore \; \frac{A(E)}{2\pi} = i\left(\frac{1}{E - \varepsilon' + \frac{i\gamma}{2}} - \frac{1}{E - \varepsilon' - \frac{i\gamma}{2}}\right)$$

$$= \frac{\gamma}{(E - \varepsilon')^2 + \left(\frac{\gamma}{2}\right)^2} = D(E)$$

Note: $D(E) = 1/2\pi$ Trace$[A(E)]$ in general, and for a 1-level device $D(E)=A(E)/2\pi$

- This is exactly the 1-level device DOS Lorentzian broadening discussed at the beginning of the course!

Lorentzian



- Thus, the overall broadening effect (and lifetime) is described by the self-energy, $\Sigma(E)$

- Next time: the role of $\pm i0^{+}$