Fundamentals of Nanoelectronics

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11.15.2004

Lecture 32: Broadening and Lifetime

Ref. Chapter 8.1

Network for Computational Nanotechnology

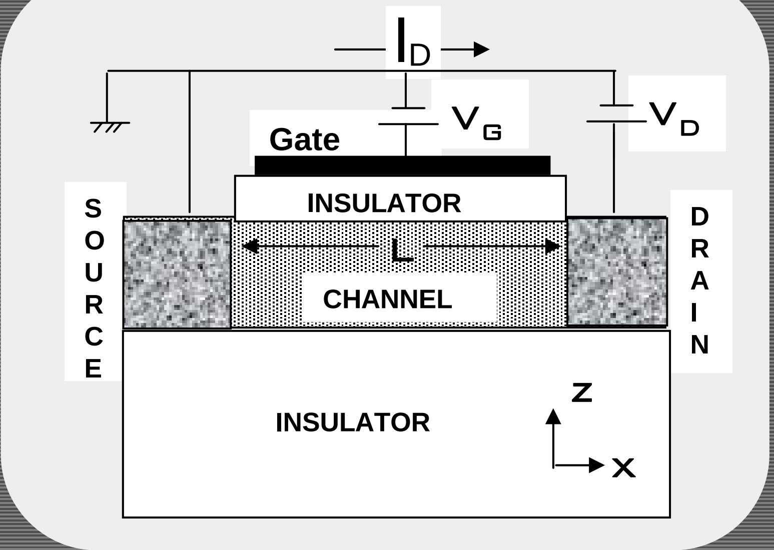
NCN nanoHUB online simulations and more

Overview

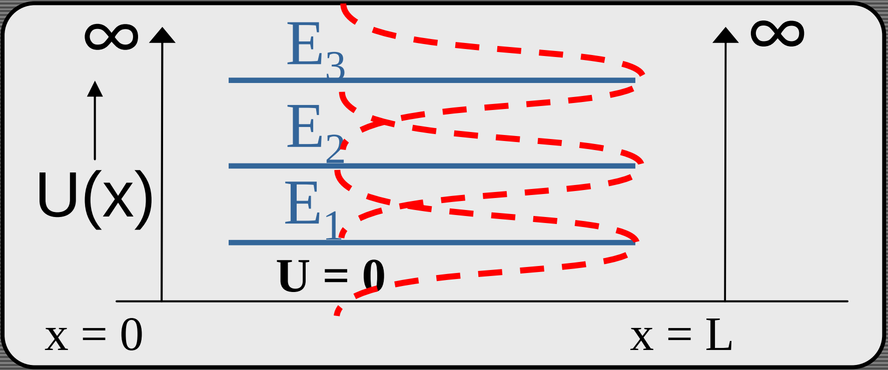
00:03

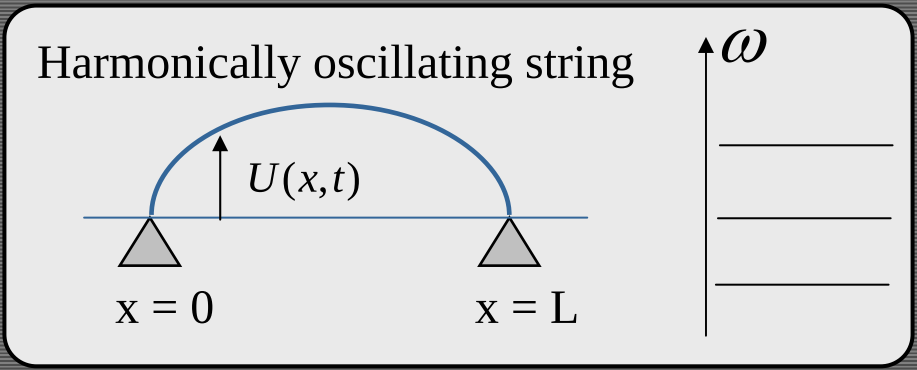
• So far we've been discussing closed systems. For closed systems the governing equation is $\left[EI - H\right]\{\Psi\} = \{0\} \quad (1)$ the eigenvalues of H give us the energy levels of the device. But in general any practical device will involve current flow and then the system will be an open one. What we like to know is that how easily electrons can get into the channel and how easily the can get out.

Field Effect Transistor



Review





- Schrödinger equation is a wave equation. A common example of a wave equation is the acoustic waves on a string. There the quantity that is used to describe the wave is the displacement of each point on a string from an equilibrium point at a particular time. In the case of Schrödinger equation this would be the allowed energy levels.
- The problem we are trying to understand today is analogous to the plucking the guitar string and investigating the frequencies at which it vibrates.
- In our case we are hitting the channel with electrons from the contact. What we like to understand is the change to the energy levels in the channel which were the energy levels of a particle in a box prior to being hit by electrons. In other words we are interested in the excitation of the channel due to contact. This change in the problem results in the following change in the Schrödinger equation:

$$[EI - H]\{\Psi\} = \{0\} \rightarrow [EI - H - \Sigma]\{\Psi\} = \{S\}$$

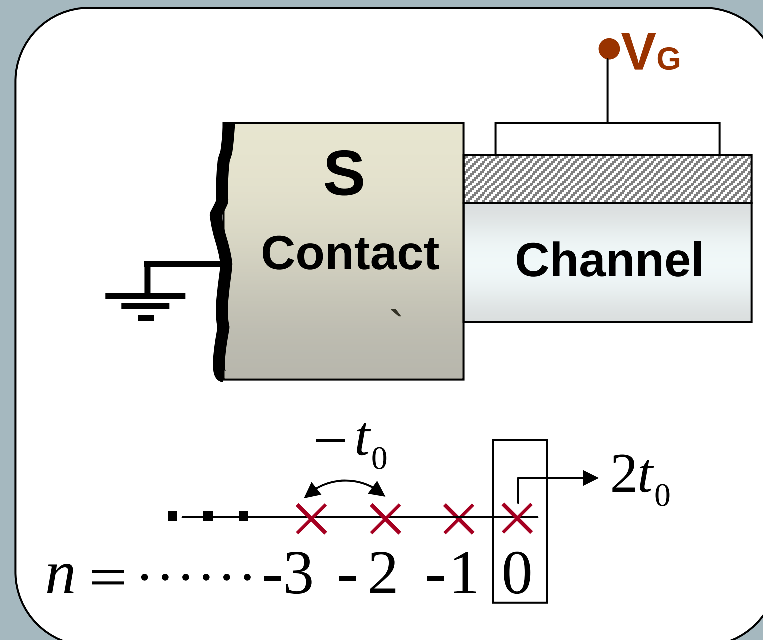
Review

03:45

- What we've seen last time is that starting from Schrödinger equation, we could eliminate the source contact and come up with:

$$\left[EI - H - \Sigma\right]\left\{\Psi\right\} = \left\{S\right\}$$

$$E\phi_0 = \underbrace{2t_0}_{H}\phi_0 \underbrace{- t_0 e^{ika}}_{\Sigma}\phi_0 \underbrace{- t_0 B\left(e^{-ika} - e^{+ika}\right)}_{S}$$



- Here, H describes the channel. Sigma describes the surrounding. "S" is the source term which tells us how electrons are getting into the channel. "S" is what drives the channel. psi is the response of the channel to the excitation by the contact. DOS tells us how well the channel responds at a given energy.

Effect of Contact on the Channel

$$[EI - H - \Sigma]\{\Psi\} = \{S\} \quad (1)$$

- To show the effect of source in the wave function in the channel we can rewrite equation (1) as:

$$\{\psi\} = [G]\{S\}$$

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

- A nice observation is that, if energy E matches one of the energy levels in H, then the matrix G tends to be large. Since psi is given as the matrix product of G and S, there is significant response from the channel and that is reflected in psi.
- The self energy term Σ has two aspects to it: one is the broadening and the other is the finite lifetime of a given state in contact. And these are what we want to talk about today.

Open System

07:15

- Let's review how we got from equation 1 to 2:

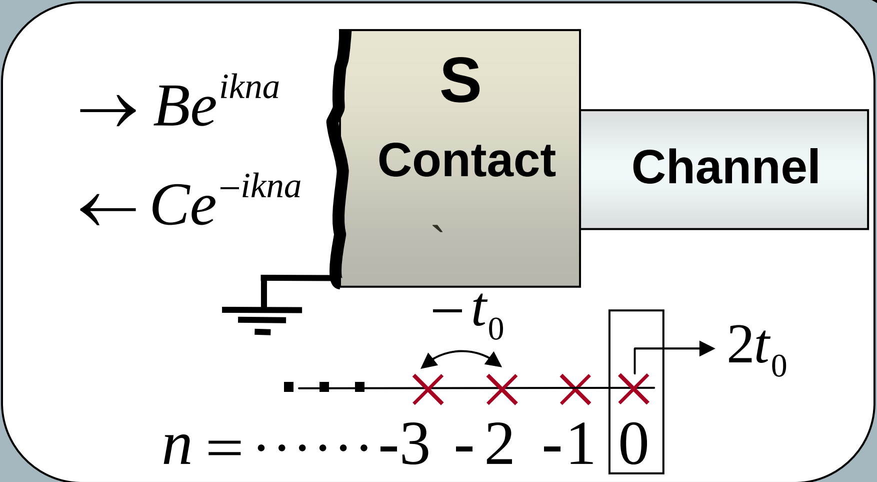
$$[EI - H]\{\Psi\} = \{0\} \quad (1)$$

$$[EI - H - \Sigma]\{\Psi\} = \{S\} \quad (2)$$

- Let's write the over Hamiltonian for combination of channel and contact.

$$\begin{array}{cc} & \begin{array}{cc} \textbf{Source Contact} & \textbf{Ch.} \end{array} \\ [\overline{H}] = & \left[\begin{array}{cccc|c} \ddots & & & & \\ & \ddots & & & \\ & & 2t_0 & -t_0 & \\ & & -t_0 & 2t_0 & -t_0 \\ \hline & & & & 2t_0 \end{array}\right] \end{array}$$

$$\boxed{t_0 = \hbar^2 / 2ma^2}$$



- In terms of the overall Hamiltonian and the continuum of energies we can write Schrödinger equation as: $\left(E\overline{I} - \overline{H}\right)\overline{\psi} = 0$
- The wavefunction in the source contact can be written as: $\phi_n = Be^{ikna} + Ce^{-ikna}$
- Using the solution above and through some algebra we eliminated the source contact part of Hamiltonian and we derived equation 2 where:

$$H = 2t_0 \qquad S = t_0 B\left(e^{ika} - e^{-ika}\right)$$
$$\Sigma = -t_0 e^{ika}$$

Source Term: Physical Interpretation

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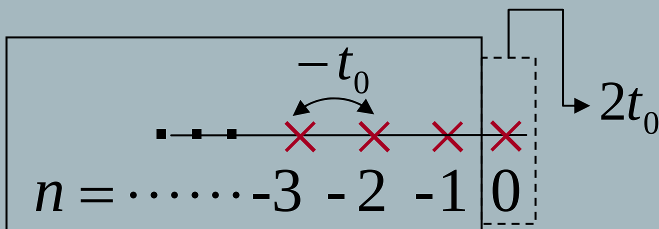


$$\boxed{S = -t_0 B\left(e^{-ika} - e^{+ika}\right)}$$

- What multiplies t0 is the wavefunction that we'd have at point -1 if we'd completely disconnected it from the device (channel).
- This comes from the boundary condition that wavefucntion has to be 0 at point 0.

$$\phi_n = Be^{ikna} + Ce^{-ikna} \begin{cases} \phi_0 = B + C \\ \phi_{-1} = Be^{-ika} + Ce^{+ika} = \cancel{e^{+ika}\phi_0} + \left(Be^{-ika} - Be^{+ika}\right) \end{cases}$$

0 (disconnected from channel)

- When the contact and channel are connected together the response of the channel can bed written as:

$$\left[EI - H - \Sigma\right]\left\{\Psi\right\} = \left\{S\right\} \longrightarrow \left\{\psi\right\} = \left[G\right]\left\{S\right\}$$

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

Finite Lifetime Aspect of Σ

- Next we'd like to explain how Σ is related to lifetime.
- Let's start with Schrödinger equation: (suppose the channel is isolated form the contact)

$$i\hbar\frac{d\psi}{dt}=H\psi,\ \text{Let}\ H=\varepsilon,\ \text{then}\,\psi(t)\ \text{can be written as}\ \psi(t)=\psi(0)e^{\frac{-i\varepsilon}{\hbar}t}$$

- Remember that we described the effect of the contact by the term Σ . If add this to H we get:

$$i\hbar\frac{d\psi}{dt}=H\psi;H=\varepsilon+\Sigma,\ \text{then}\ \psi(t)=\psi(0)e^{\frac{-i\varepsilon}{\hbar}t}e^{\frac{-i\Sigma}{\hbar}t}$$

- If Σ is real, then there has been a shift in the energy and not much has changed. But if Σ has an imaginary part, then a DECAY factor is involved.

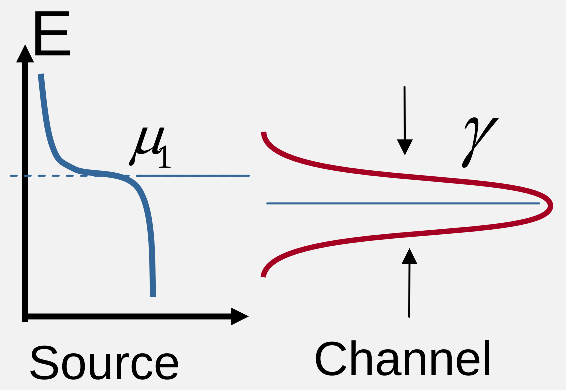
$$\left.\begin{aligned}\psi(t)&=\psi(0)e^{\frac{-i\varepsilon}{\hbar}t}e^{\frac{-i\Sigma}{\hbar}t}\\ \varepsilon'&=\varepsilon+\mathrm{Re}\ \Sigma\\ \gamma/2&=-\mathrm{Im}\ \Sigma\end{aligned}\right\}\psi(t)=\psi(0)e^{\frac{-i\varepsilon'}{\hbar}t}e^{-\frac{\gamma}{2\hbar}t}\Rightarrow|\psi(t)|^2=|\psi(0)|^2e^{-\gamma t/\hbar}$$

- The electron density is the magnitude of psi^2 (see above). The expression for electron density shows the significance of the imaginary part of Σ . If there is not a coupling between the contact and channel the electron density remains constant. But if there is an imaginary part, the electron density has finite lifetime and it decays with time.

Broadening Aspect of Σ

• We just learned that the imaginary part of Σ results in a finite lifetime. Another aspect of this is broadening. Early on in the course we discussed that if we connect the channel to a contact then, then the levels in the channel gets broadened. We stated that the a single sharp energy level looses a fraction of its value but then some fraction of energy levels from the contact spill over in the channel. As the result we had a broadening. The important point was that what the channel level looses at a particular energy, it gains the same amount at other energies so that the sum of the new distribution of energy levels adds up to 1 which is the value it had before connecting the channel to the contact.

• It is very important to keep broadening in the whole picture. Without it the value of calculated current will be wrong.



Broadening

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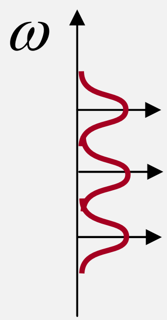
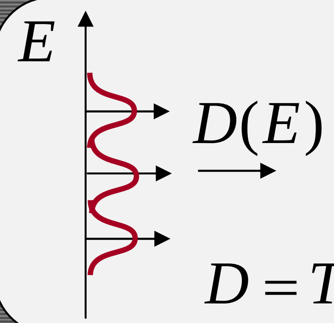


Resonant Frequencies and Broadening



$$D = Trace\left(i(G - G^{+})/2\pi\right)$$

- Consider a guitar string with certain resonant frequencies. If we hit the we expect to see a response where the sharp frequencies are broadened.
- The ides is the same for our discussion. As long as we have a governing equation like:

$$\left(EI - H\right)\psi = 0$$

- we have infinite response at specific energies.
- Once we have something like:

$$\left(EI - H - \Sigma\right)\psi = S$$

the response will be broadened.

- For our model the response that includes broadening can be written as:

$$\{\psi\} = [G]\{S\}$$

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

- So the amplitude of the response can be written as the G matrix denoted above. If G is large then the source excites a big response and if it is small, the source doesn't excite much.
- Notice that the formula for D requires more discussion which comes later for now if we accept it, then…

Broadened DOS For 1 level

- What would DOS be if we have a state with: $H=\varepsilon \qquad \Sigma=\sigma-\frac{i\gamma}{2}$

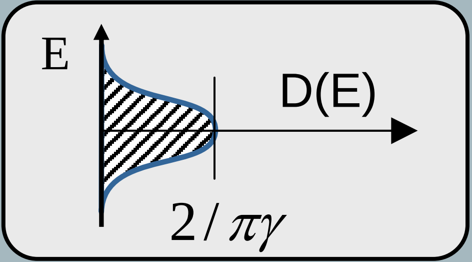
$$G=\frac{1}{E-\varepsilon-\sigma+\frac{i\gamma}{2}}=\frac{1}{E-\varepsilon'+\frac{i\gamma}{2}} \qquad \varepsilon+\sigma\equiv\varepsilon'$$

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

$$D(E)=\frac{i}{2\pi}Trace\big((G-G^{+})\big)=\frac{i}{2\pi}\left(\frac{1}{E-\varepsilon'+\frac{i\gamma}{2}}-\frac{1}{E-\varepsilon'-\frac{i\gamma}{2}}\right)=\frac{i}{2\pi}\left(\frac{-i\gamma}{(E-\varepsilon')^2+\left(\frac{\gamma}{2}\right)^2}\right)$$

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

Lorentzian distribution describing the broadening of a ←level→



Summary

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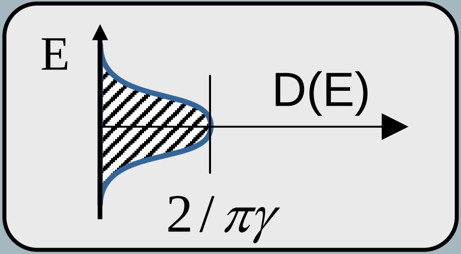
• To sum up note that when dealing with closed system we deal with a Schrödinger equation like:

$$\left[EI - H\right]\left\{\Psi\right\} = \left\{0\right\} \quad (1)$$

• But for any problem that involves current flow we have to consider an open system:

$$\left[EI - H - \Sigma\right]\left\{\Psi\right\} = \left\{S\right\} \quad (2)$$

• In (2), H describes the channel. Sigma describes the surrounding. “S” is the source term which tells us how electrons are getting into the channel. psi is the response of the channel to the excitation by the contact. DOS tells us how well the channel responds at a given energy.



For weak coupling the channel only responds at certain sharp energies. For strong coupling the levels broaden out and the channel responds at more energy values because of broadening.

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