Fundamentals of Nanoelectronics

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Lecture 31: Broadening

Ref. Chapter 8.1

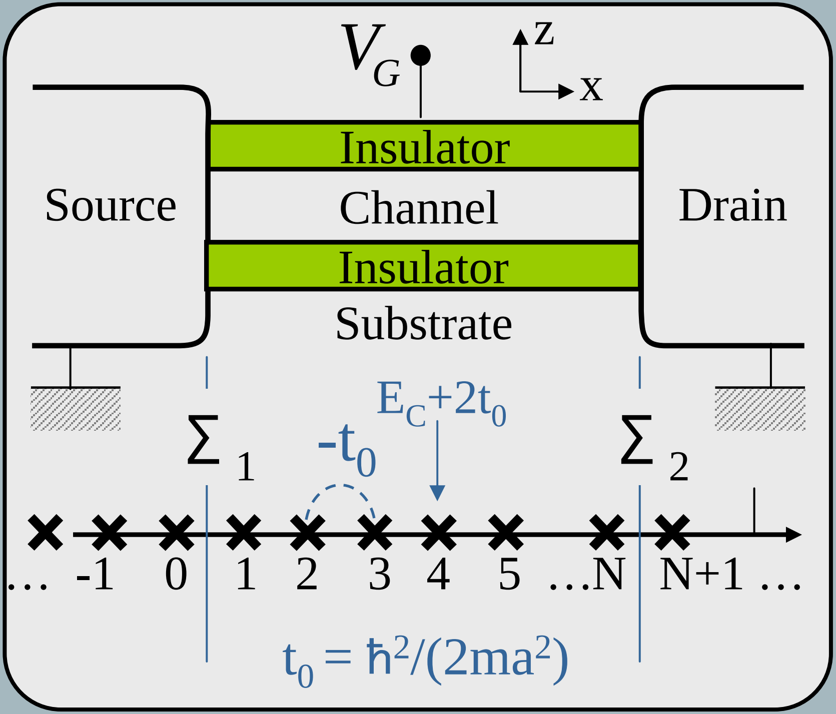
Network for Computational Nanotechnology

NCN nanoHUB online simulations and more

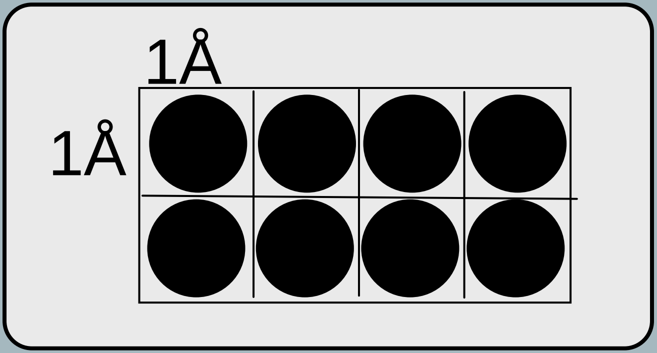
Review

00:03

• Our goal in this course is to calculate the current through a small device:



• Last time we discussed the change in the electron density due to the gate voltage. As VG changes the levels in the channel move up and down.



• How large is the number of added electrons per cm^2 if we add one to each atom?

$$n_{added} = 10^{16}\,/\,cm^2$$

• So if the gate voltage adds 10^12/cm^2, that number is relatively small because it adds 1 electron every 100 Å by 100 Å.

Overview

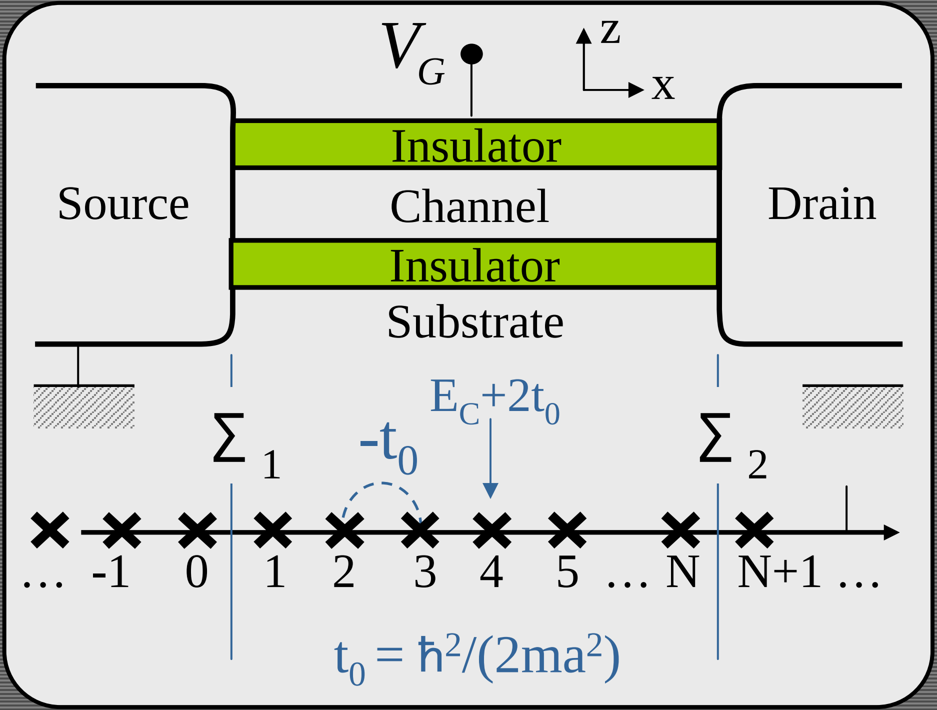
04:40

- Today we'd like to discuss broadening. Up till now we've been talking about isolated structures:

$$E\{\Psi\} = [H]\{\Psi\}$$

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

- But if we consider open systems, we have to know what broadening does in order to calculate current.



Broadening: Importance

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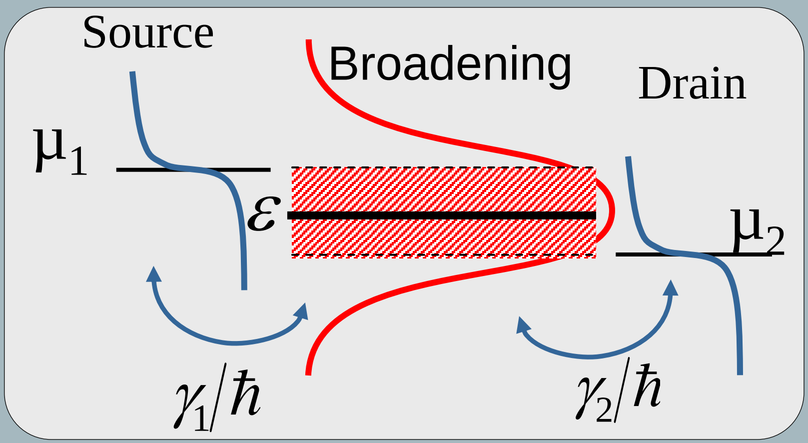
Broadening of a level



At the beginning of the course we discussed broadening. There it was mentioned that if broadening wasn't taken into account then the calculated current wouldn’t be right and not saturate.

• However if we include broadening, the some part of the broadened level lies outside of the range between mu1 and mu2; hence it that part will not contribute to the current and the current saturates.

• Maximum current was given as:

$$I \propto \frac{2q^2}{h} V$$

• We calculated the current to be:

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

• Broadening included, we had:

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

Broadening: Importance

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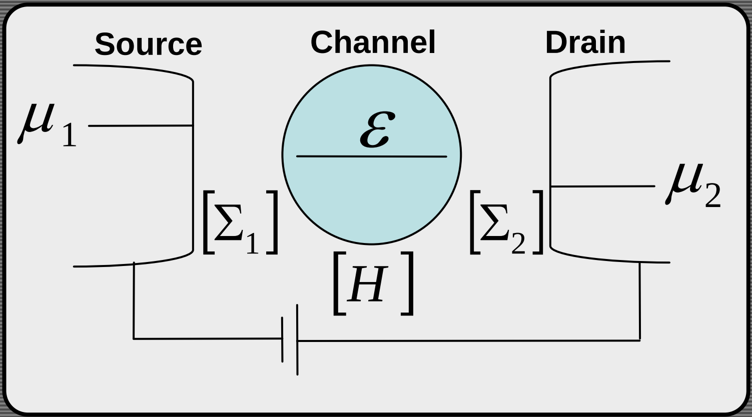
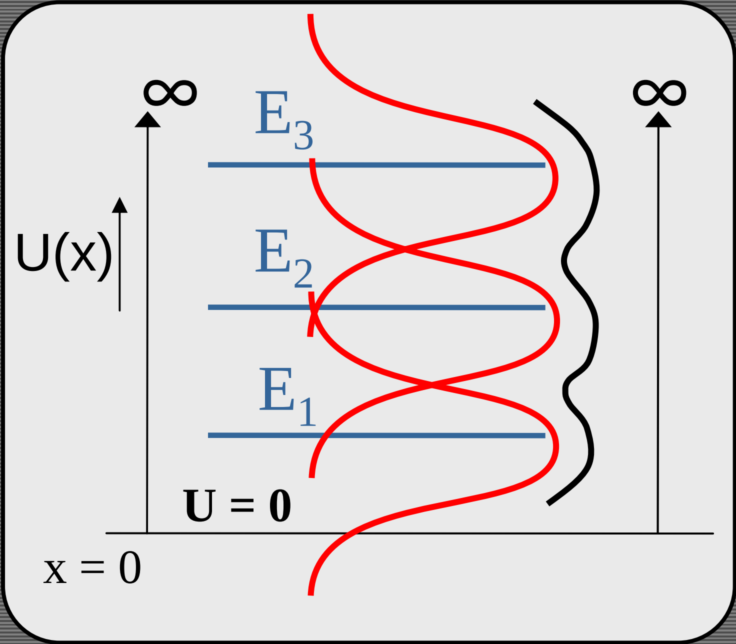
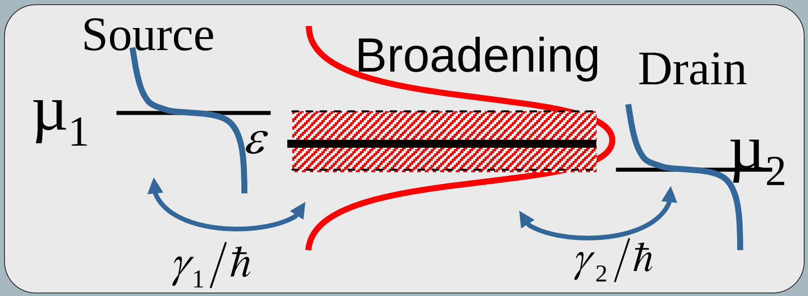




- The concept of broadening is also very important for small devices. As the channel is made smaller and smaller, the levels become discretized. The spacing between them depends on the length of the channel: L.. The shorter the channel, the larger the spacing. If the spacing is bigger than kT, then the expectation is that it will have significant effect on observables. For small transistors with very good contacts however this has not been the case. This is due to the significant broadening of the levels because of good connection to contacts which negates the effect of spacing. (As the figure shows broadening of the levels makes them closer together.) How ever one can see observable effects if the contacts are connected poorly.



Isolated System

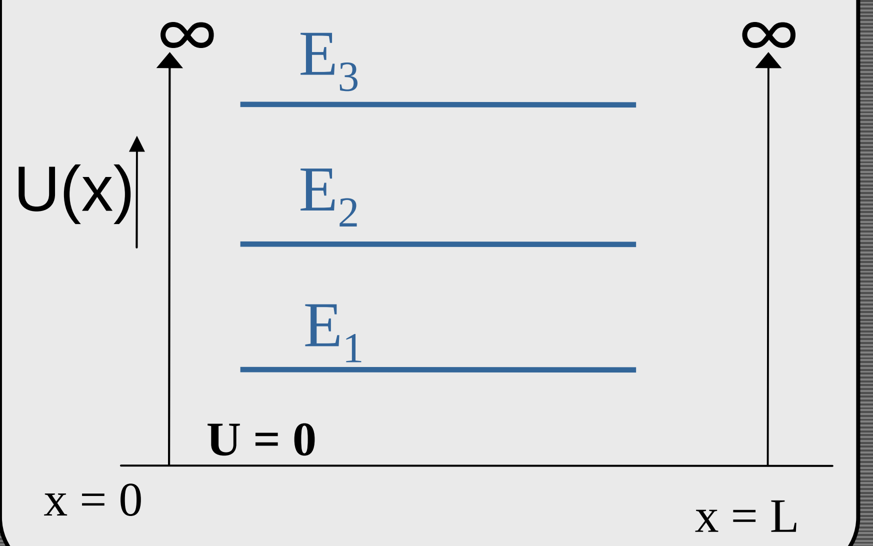
- To start, think of an isolated system. The matrix version of Schrödinger equation reads:

$$E\{\Psi\} = [H]\{\Psi\} \quad (1)$$

- (1) can be written as:

$$[EI - H]\{\Psi\} = \{0\} \quad (2)$$

- The only non trivial (non zero) wavefunction solution to (2) happens when the matrix that multiplies psi on the left is singular, i.e. it does not have an inverse.
- For the box problem, electrons can only exist on the discrete energy levels.



Channel and a Contact

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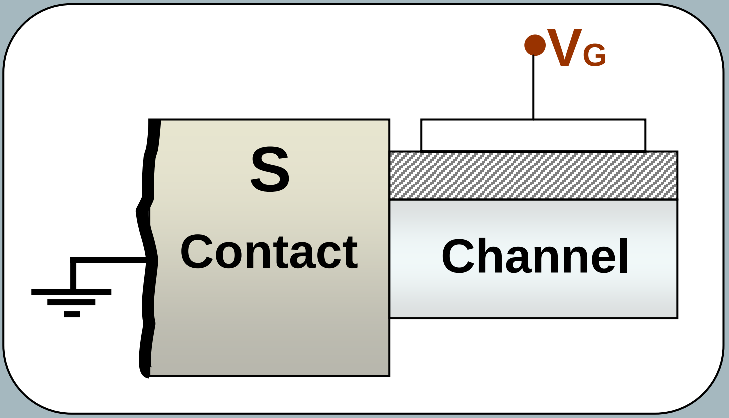

• In this the electrons can from a continuum of allowed states in the contact want to get into the channel. The governing equation for the channel can now be written as:

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

From Contact

Schrödinger Equation / Wave Equation

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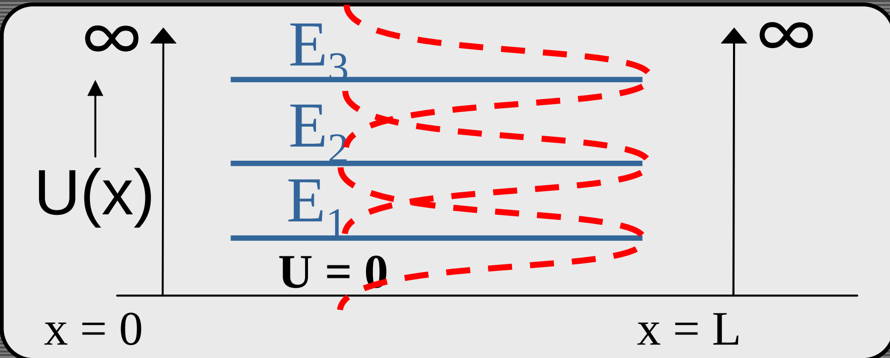
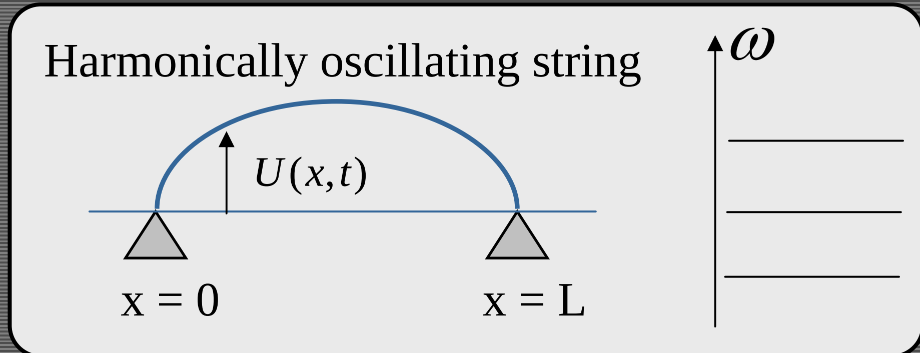
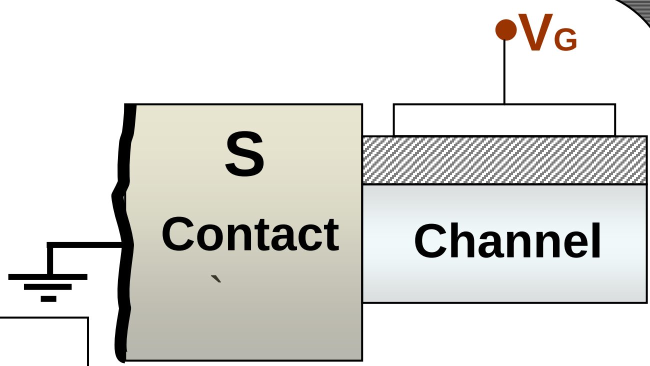




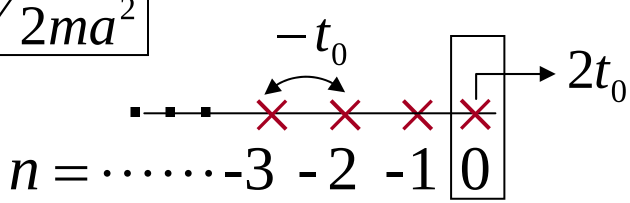
- Schrödinger equation is a wave equation. A common example of a wave equation is the acoustic waves on a string. There the quantity that is used to describe the wave is the displacement of each point on a string from an equilibrium point at a particular time. In the case of Schrödinger equation this 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:

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

Broadening: A Simple Example



$$t_0 = \hbar^2 / 2ma^2$$



$$E\{\Psi\} = [H]\{\Psi\}$$

$$E\phi_0 = 2t_0\phi_0 - t_0\phi_{-1} : \text{1st Equation}$$

$$E\phi_{-1} = -t_0\phi_{-2} + 2t_0\phi_{-1} - t_0\phi_0$$

$$E\phi_n = t_0\left(-\phi_{n-1} + 2\phi_n - \phi_{n+1}\right) : nth \text{ Eq.}$$

- The following forms of solution will satisfy the nth equation:

$$\phi_n = e^{ikna} \quad \text{or} \quad e^{-ikna}$$

- Provided the following E-k relation holds: (use the nth Eq. to find E in terms of k)

$$\frac{\phi_{n+1}}{\phi_n} = e^{+ika} \qquad \frac{\phi_{n-1}}{\phi_n} = e^{-ika}$$

$$E = t_0(e^{-ika} + 2 - e^{+ika}) = 2t_0(1 - \cos ka)$$

- The general solution can be written as:

$$\phi_n = Be^{ikna} + Ce^{-ikna}$$

Broadening: Example Continued

$$E\phi_0 = 2t_0\phi_0 - t_0\phi_{-1} : \text{1st Equation}$$

• We want to get rid of phi_-1 term in the first equation and replace it with a Σ that describes the effect of the contact on the channel. To do this start with the general solution:

$$\phi_n = Be^{ikna} + Ce^{-ikna} \begin{cases} \phi_0 = B + C \\ \phi_{-1} = Be^{-ika} + Ce^{+ika} = e^{+ika}\phi_0 + (Be^{-ika} - Be^{+ika}); \; (2) \end{cases}$$

• Substitute (2) in the 1st Equation→ $E\phi_0 = 2t_0\phi_0 - t_0 e^{ika}\phi_0 - t_0 B\left(e^{-ika} - e^{+ika}\right)$ (3)

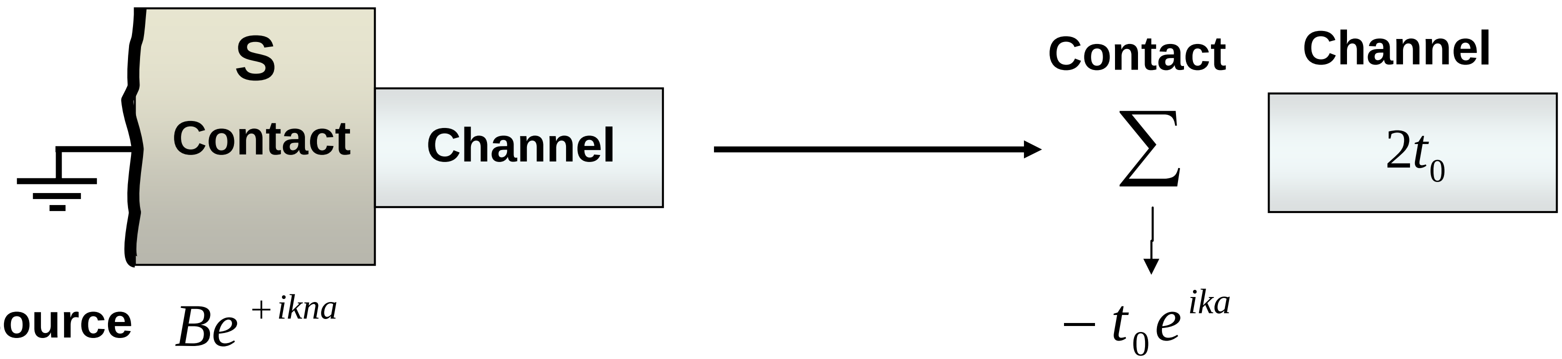
• If the channel was isolated from the contact we'd have: $E\phi_0 = 2t_0\phi_0$

• With connection to the contact we have additional terms (Equation 3) which can be grouped and denoted as:

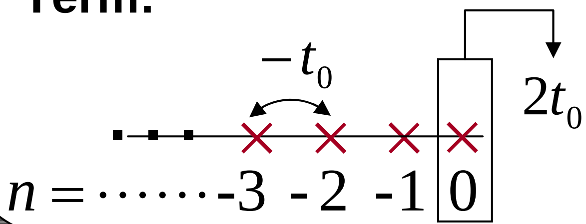
$$E\phi_0 = \underbrace{2t_0}_{H}\phi_0 \underbrace{- t_0 e^{ika}}_{\Sigma}\phi_0 \underbrace{- t_0 B\left(e^{-ika} - e^{+ika}\right)}_{S}$$

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

Broadening: Physical Picture



Source Term: Be^{+ikna}



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

- One main difference between H and Σ is that the diagonal elements of Σ are complex in general whereas H has real values for its diagonal elements because it has to be Hermitian.

$$H = \begin{bmatrix} 2t_0 & & \\ & \ddots & \\ & & \end{bmatrix} \qquad \Sigma = \begin{bmatrix} -t_0 e^{ika} & & \\ & \ddots & \\ & & \ddots \end{bmatrix}$$

Broadening: Physical Picture

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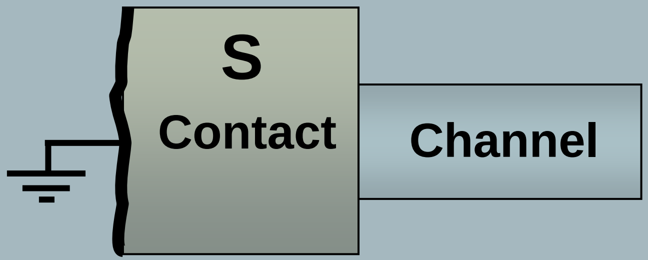
• We can define a broadening matrix as the imaginary part of Σ:

$$\Gamma = i(\Sigma - \Sigma^{+}) = i(-t_0 e^{ika} + t_0 e^{-ika}) = 2t_0 \sin ka$$

• Physically, gamma represents the effect of connecting the channel to the semi-infinite contact. In the contact we have the dispersion relation: $E = 2t_0(1 - \cos ka)$



• And velocity can be written as: $v = \hbar \dfrac{dE}{dk}$

• This means that we can write gamma as: $\Gamma = \hbar v / a$

• An electron in the contact wants to escape from the contact with the velocity v. This way we can interpret Gamma as a measure of hot fast the electron can get out of the contact.