Physics of Semiconductors

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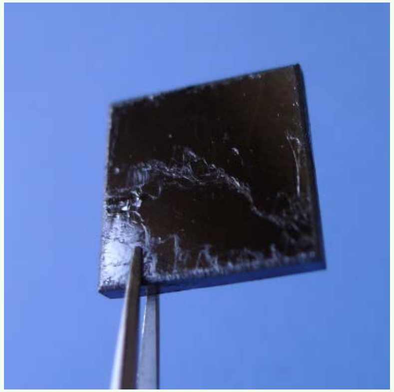
Shingo Katsumoto
Department of Physics
and
Institute for Solid State Physics
University of Tokyo

Outline today

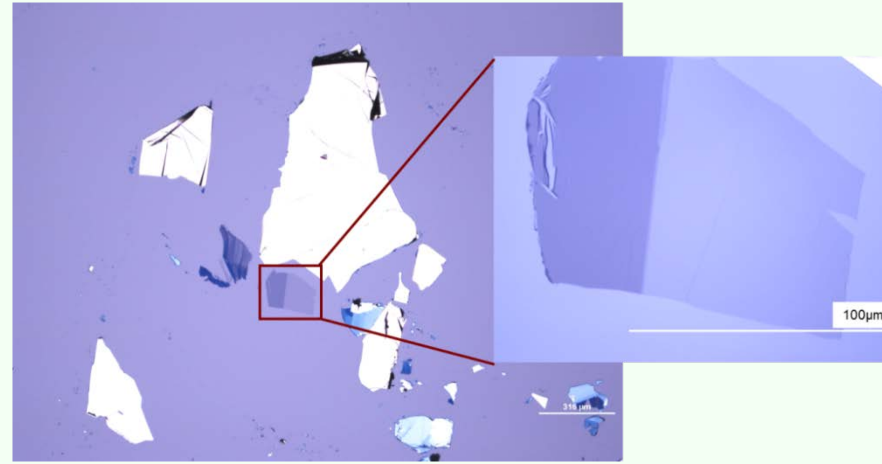
- Graphene: A two-dimensional material
- Quantum wire and fundamentals of quantum transport
  - Formation of quantum wires
  - Boundary between classical and quantum
  - Landauer formula
    - Quantized conductance
    - Quantum point contact and conductance channel
    - S-matrix
    - Onsager reciprocity
  - Landauer-Büttiker multi-probe formula

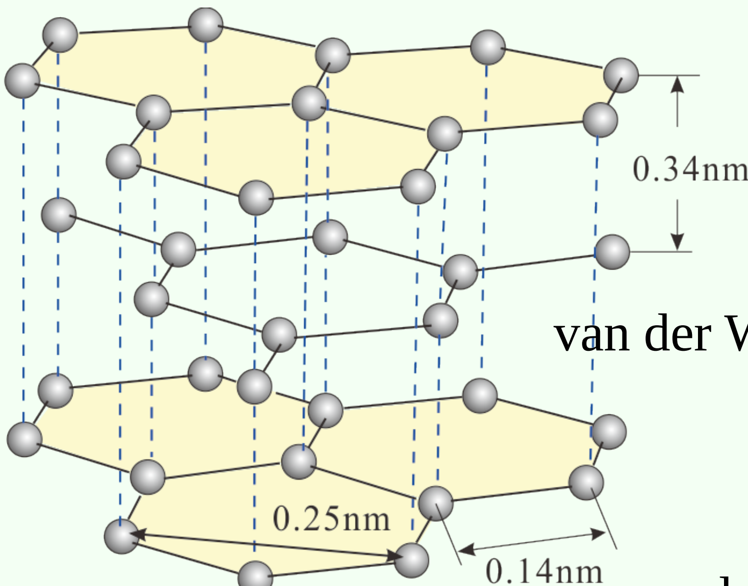
Graphene: A two-dimensional material

Graphite



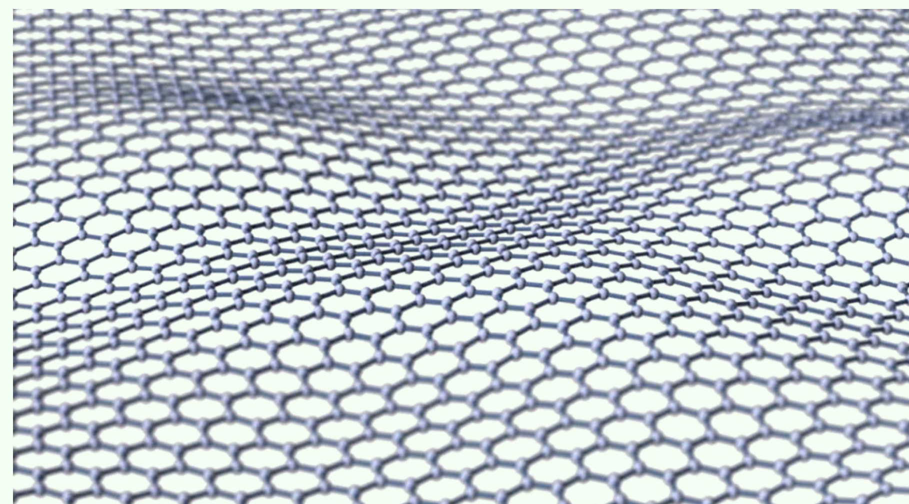
Graphene





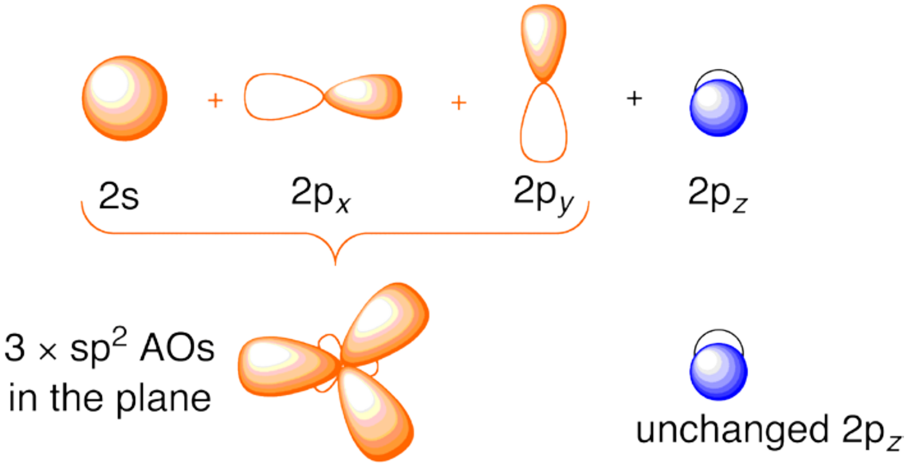
van der Waals

covalent

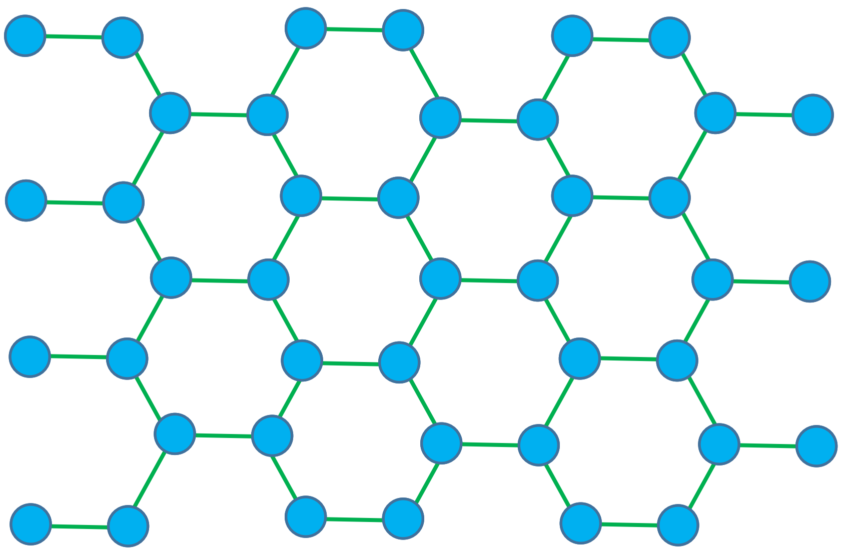


Graphene lattice/reciprocal lattice structure

Atomic orbitals

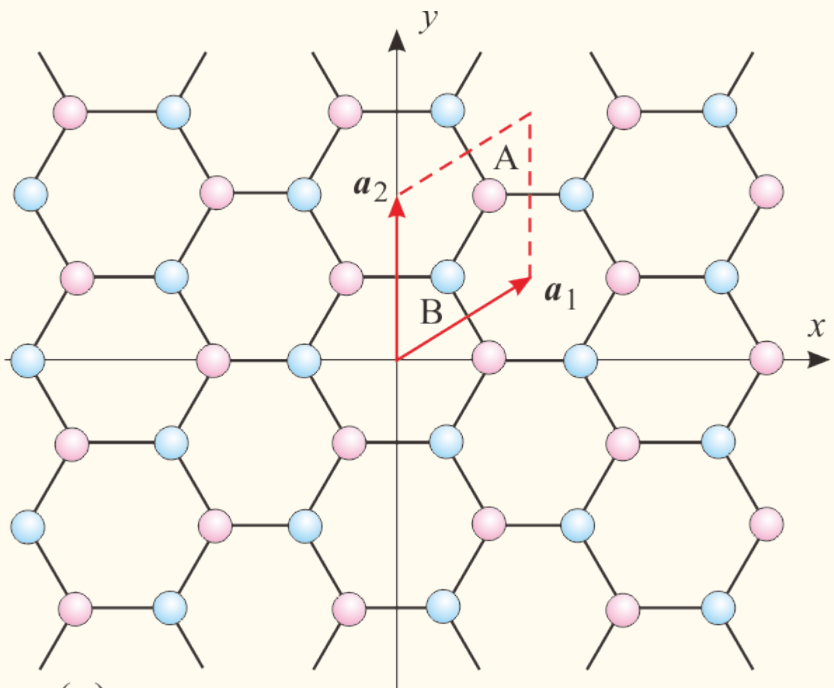


Honeycomb lattice



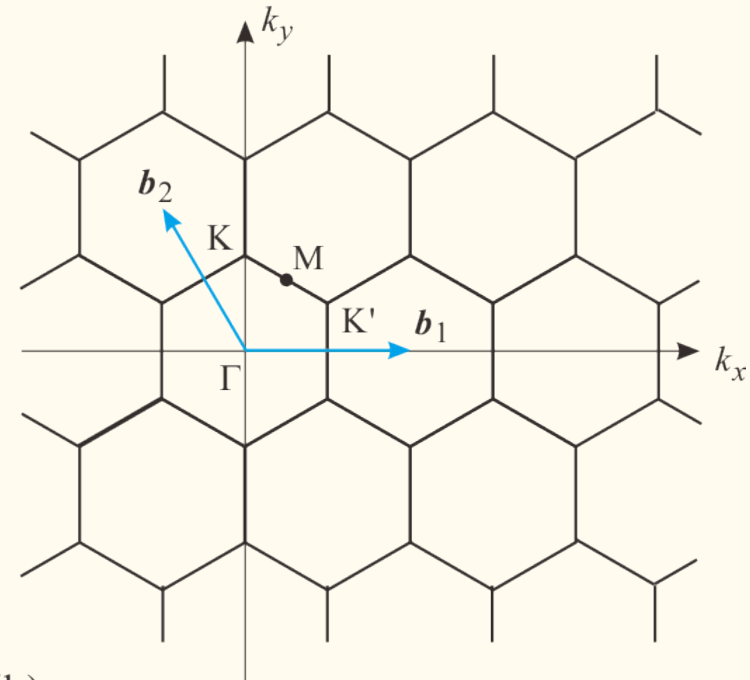
Graphene lattice/reciprocal lattice structure

Lattice: unit cell



(a)

Reciprocal lattice



(b)

$$\boldsymbol{a}_1 = \begin{pmatrix} \sqrt{3}a/2 \\ a/2 \end{pmatrix}, \quad \boldsymbol{a}_2 = \begin{pmatrix} 0 \\ a \end{pmatrix}$$

$$\boldsymbol{b}_1 = \begin{pmatrix} 4\pi/\sqrt{3}a \\ 0 \end{pmatrix}, \quad \boldsymbol{b}_2 = \begin{pmatrix} -2\pi/\sqrt{3}a \\ 2\pi/a \end{pmatrix}$$

Tight binding model

$$\psi = \zeta_{\mathrm{A}}\psi_{\mathrm{A}} + \zeta_{\mathrm{B}}\psi_{\mathrm{B}} \qquad \langle\psi_{\mathrm{A}}|\psi_{\mathrm{A}}\rangle = \langle\psi_{\mathrm{B}}|\psi_{\mathrm{B}}\rangle = N$$

$$\psi_{\mathrm{A}} = \sum_{j\in A}\exp(i\boldsymbol{k}\boldsymbol{r}_j)\phi(\boldsymbol{r}-\boldsymbol{r}_j), \quad \psi_{\mathrm{B}} = \sum_{j\in B}\exp(i\boldsymbol{k}\boldsymbol{r}_j)\phi(\boldsymbol{r}-\boldsymbol{r}_j).$$

$$H_{\mathrm{AA}} = \langle\psi_{\mathrm{A}}|\mathscr{H}|\psi_{\mathrm{A}}\rangle, \quad H_{\mathrm{BB}} = \langle\psi_{\mathrm{B}}|\mathscr{H}|\psi_{\mathrm{B}}\rangle, \quad H_{\mathrm{AB}} = H_{\mathrm{BA}}^{*} = \langle\psi_{\mathrm{A}}|\mathscr{H}|\psi_{\mathrm{B}}\rangle,$$

Tight binding:

$$\langle\psi_{\mathrm{A}}|\psi_{\mathrm{B}}\rangle = 0$$

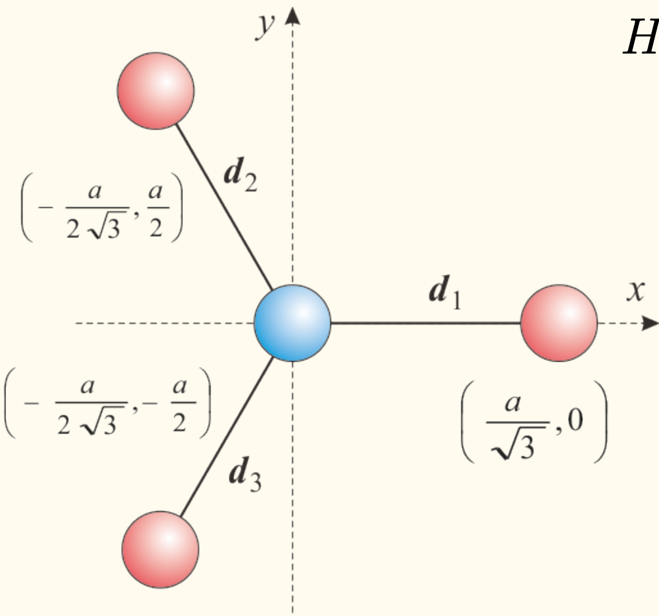
$$\mathscr{H}\psi = \begin{pmatrix} H_{\mathrm{AA}} & H_{\mathrm{AB}} \\ H_{\mathrm{BA}} & H_{\mathrm{BB}} \end{pmatrix}\begin{pmatrix} \zeta_{\mathrm{A}} \\ \zeta_{\mathrm{B}} \end{pmatrix} = NE\psi = NE\begin{pmatrix} \zeta_{\mathrm{A}} \\ \zeta_{\mathrm{B}} \end{pmatrix}$$

Eigenvalues:

$$E = \frac{1}{2N}\left(H_{\mathrm{AA}} + H_{\mathrm{BB}} \pm \sqrt{(H_{\mathrm{AA}} - H_{\mathrm{BB}})^2 + 4|H_{\mathrm{AB}}|^2}\right)$$

$$= \frac{H_{\mathrm{AA}}}{N} \pm \frac{|H_{\mathrm{AB}}|}{N} \equiv h_{\mathrm{AA}} \pm |h_{\mathrm{AB}}|$$

Sublattice transition term



$$H_{\mathrm{AB}} = \sum_{l \in \mathrm{A}, j \in \mathrm{B}} \exp\left[i\boldsymbol{k}(\boldsymbol{r}_j - \boldsymbol{r}_l)\right] \langle \phi(\boldsymbol{r} - \boldsymbol{r}_l) | \mathscr{H} | \phi(\boldsymbol{r} - \boldsymbol{r}_j) \rangle_{\boldsymbol{r}}$$

Take the nearest neighbor approximation:

$$\boldsymbol{k} \cdot \boldsymbol{d}_1 = \frac{k_x a}{\sqrt{3}}, \; \boldsymbol{k} \cdot \boldsymbol{d}_2 = \left(-\frac{k_x}{2\sqrt{3}} + \frac{k_y}{2}\right) a,$$

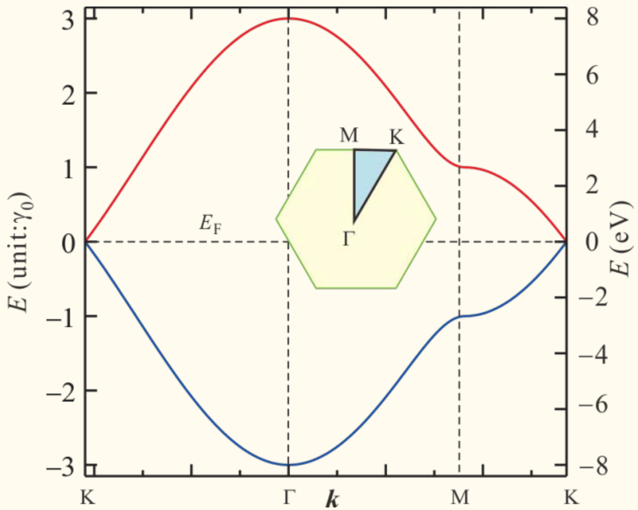
$$\boldsymbol{k} \cdot \boldsymbol{d}_3 = \left(-\frac{k_x}{2\sqrt{3}} - \frac{k_y}{2}\right) a$$

$$\langle \phi(\boldsymbol{r} - \boldsymbol{r}_l) | \mathscr{H} | \phi(\boldsymbol{r} - \boldsymbol{r}_j) \rangle_{\boldsymbol{r}} = \xi \quad \text{:constant}$$

$$|h_{\mathrm{AB}}|^2 = \left| \sum_{j=1}^{3} \exp(i\boldsymbol{k} \cdot \boldsymbol{d}_j) \right|^2 \xi^2$$

$$= \left(1 + 4\cos\frac{\sqrt{3}k_x a}{2} \cos\frac{k_y a}{2} + 4\cos^2\frac{k_y a}{2}\right) \xi^2$$

Dirac points in $\boldsymbol{k}$ -space

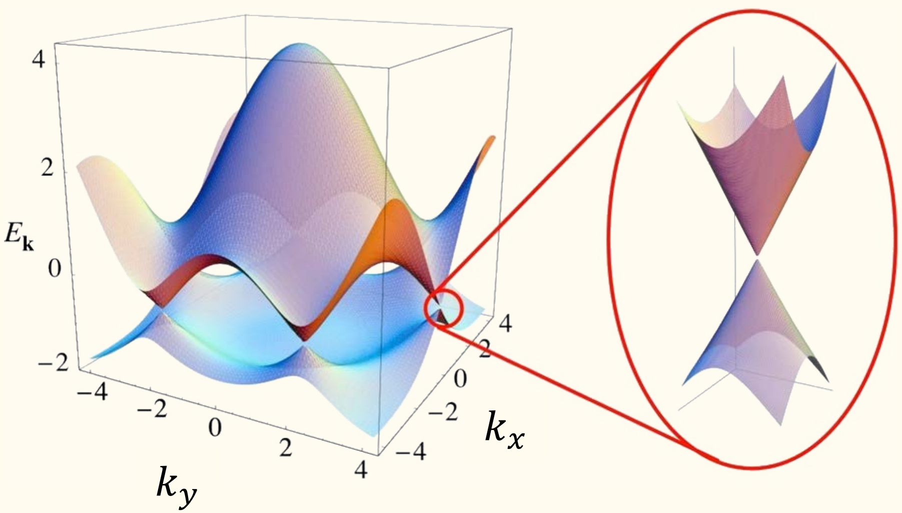


$$E = h_{\mathrm{AA}} \pm \xi \sqrt{1 + 4\cos\frac{\sqrt{3}k_x a}{2}\cos\frac{k_y a}{2} + 4\cos^2\frac{k_y a}{2}}$$

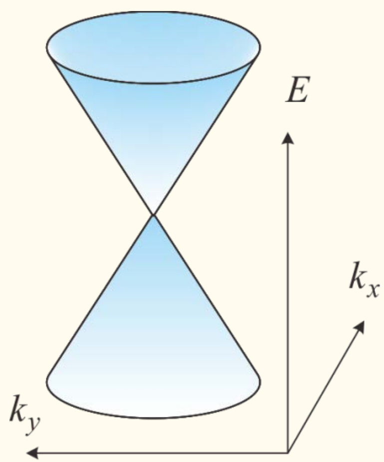
$$k_x = 0$$

$$E = h_{\mathrm{AA}} \pm \xi \left| 1 + 2\cos\frac{k_y a}{2} \right|$$

$$E\left(k_x, \frac{4\pi}{3a}\right) \approx h_{\mathrm{AA}} + \frac{\sqrt{3}\xi a}{2}|k_x|$$

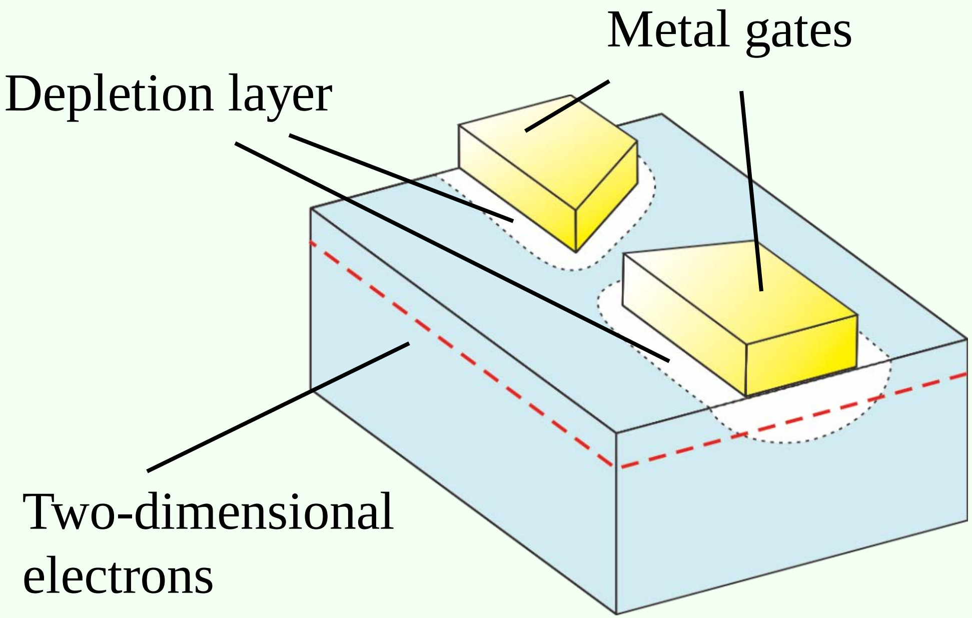


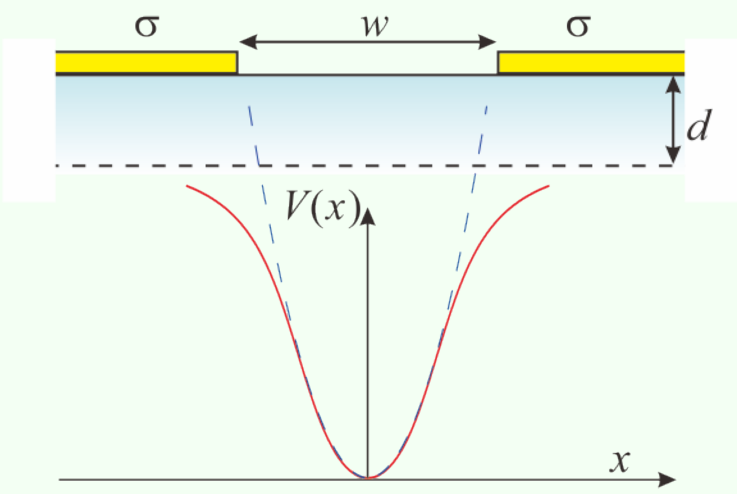
A Dirac point



Ch.4 Quantum wires
and
fundamentals of quantum transport

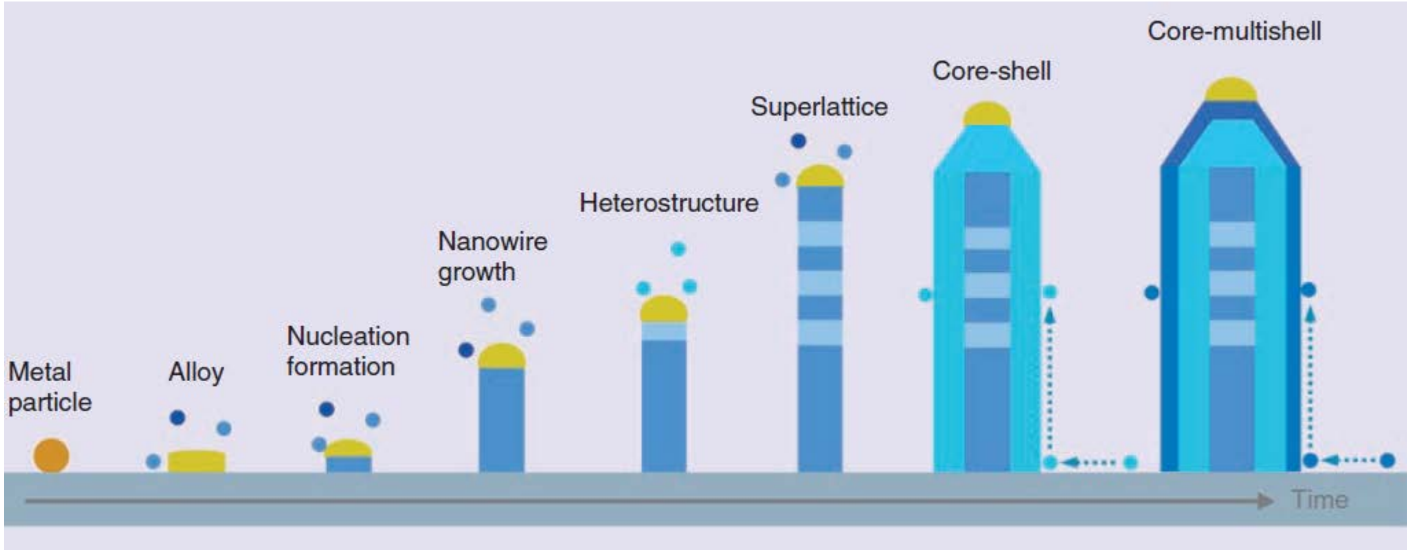
Formation of quantum wires: Split gate



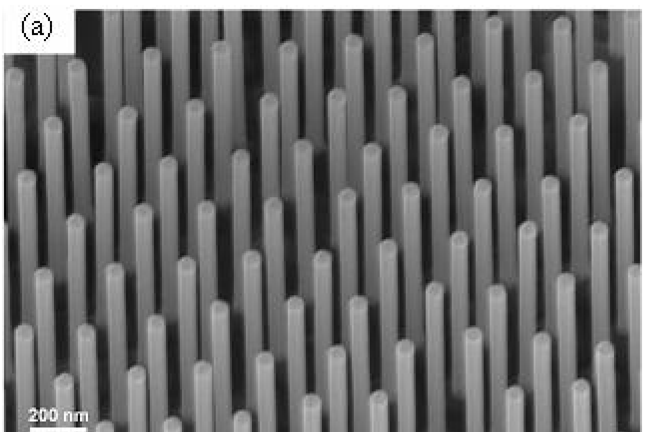


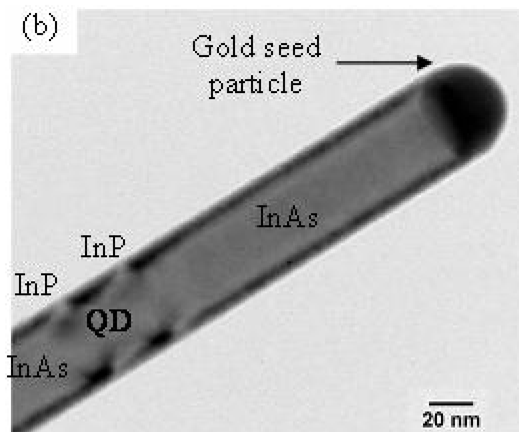
$$\mathcal{E}_z(d) = \frac{-\sigma}{2\pi\epsilon\epsilon_0}\left[\pi + \arctan\left(\frac{x - w/2}{d}\right) - \arctan\left(\frac{x + w/2}{d}\right)\right]$$

Self-assembled nano-wires



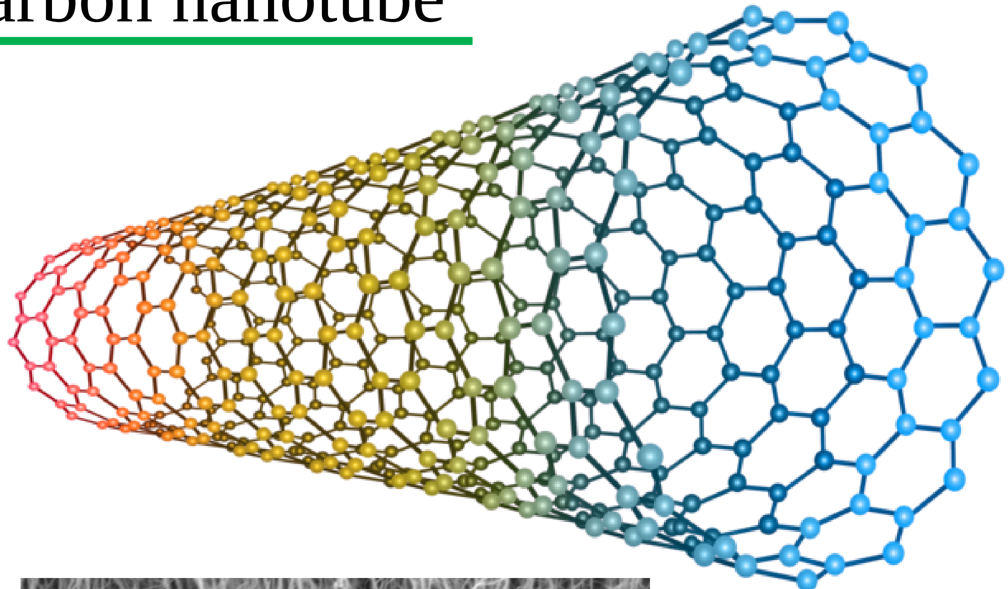
G. Zhang et al.
NTT technical Review

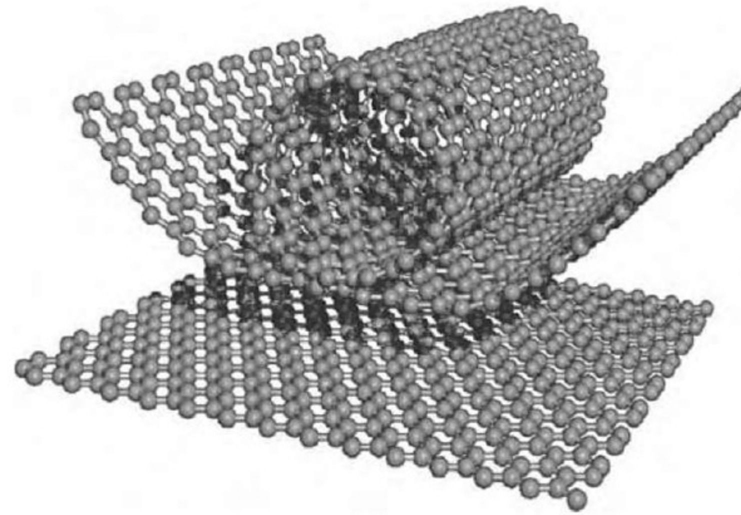


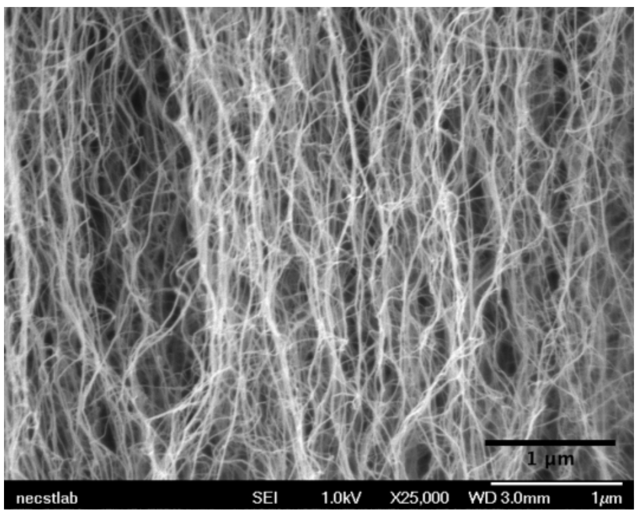


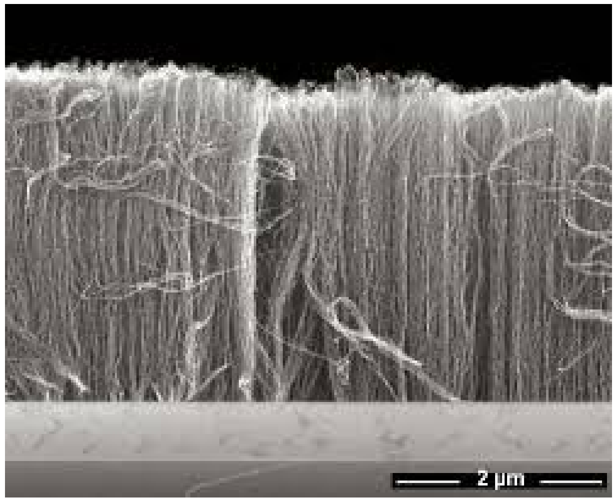
http://iemn.univ-lille1.fr/sites_perso/vignaud/english/35_nanowires.htm

Carbon nanotube

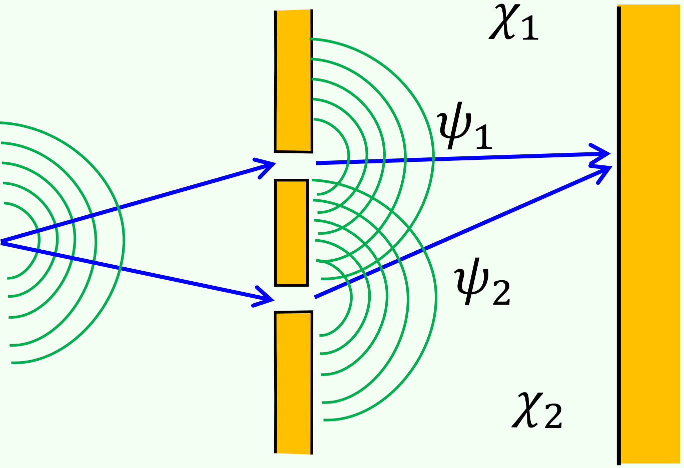








Boundary between classical and quantum



$$|\psi|^2 = |\psi_1 + \psi_2|^2$$
$$= |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2|\cos\theta$$

Environment wavefunction: χ

$$\psi_1 \rightarrow \psi_1 \otimes \chi_1, \qquad \psi_2 \rightarrow \psi_2 \otimes \chi_2$$

Interference term: $2|\psi_1||\psi_2|\cos\theta\langle\chi_1|\chi_2\rangle$

$\langle\chi_1|\chi_2\rangle = 1$: Full interference

$\langle\chi_1|\chi_2\rangle = 0$: No interference Particle-Environment maximally entangled

Electron transport: Electron – Phonon inelastic scattering
Electron – Electron inelastic scattering
Electron – Localized spin scattering

Lengths limit quantum coherence (Coherence length)

Monochromaticity: Thermal length

Energy width: $\Delta E = k_{\mathrm{B}} T$

Diffusion length: $l = \sqrt{D\tau}$

Phase width: $$2\pi \Delta f \tau = 2\pi \frac{\Delta E \tau}{h} = 2\pi \frac{k_{\mathrm{B}} T \tau}{h}$$

$$\to 2\pi : \quad \tau_c = \frac{h}{k_{\mathrm{B}} T}$$

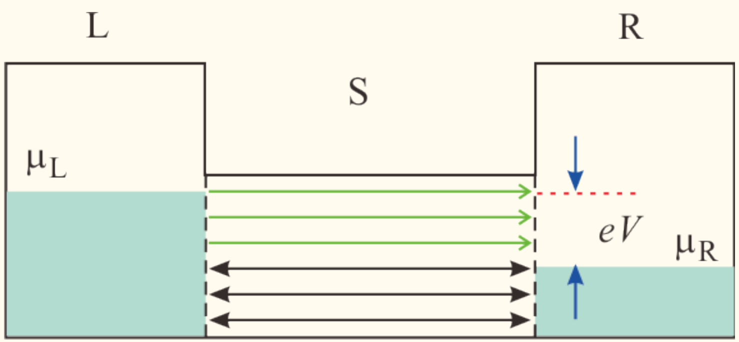
$$l_{\mathrm{th}} = \sqrt{\frac{hD}{k_{\mathrm{B}} T}}$$

Thermal diffusion length

$$l_{\mathrm{th}} = \frac{h v_{\mathrm{F}}}{k_{\mathrm{B}} T}$$

Ballistic thermal length

Conductance quantum



L, R : Particle reservoirs

Thermal equilibrium:
well defined chemical potentials

Instantaneous thermalization:
particles loose quantum coherence

$$j(k) = \frac{e}{L} v_{\mathrm{g}} = \frac{e}{\hbar L} \frac{dE(k)}{dk}$$

L: wavefunction normalization length

$$J = \int_{k_{\mathrm{R}}}^{k_{\mathrm{L}}} j(k) \frac{L}{2\pi} dk = \frac{e}{h} \int_{\mu_{\mathrm{R}}}^{\mu_{\mathrm{L}}} dE = \frac{e}{h}(\mu_{\mathrm{L}} - \mu_{\mathrm{R}}) = \frac{e^2}{h} V$$

$$G = \frac{J}{V} = \frac{e^2}{h} \equiv G_{\mathrm{q}} \text{ Conductance quantum } \left(\frac{2e^2}{h} \equiv G_{\mathrm{q}} \text{ spin freedom} \right)$$

Conductance quantum as uncertainty relation

Wave packet: $$\Delta k \to \Delta x = \frac{2\pi}{\Delta k}, \quad v_{\mathrm{g}} = \frac{\Delta E}{\hbar \Delta k}$$

Fermion statistics: electron charge concentration $$= \frac{e}{\Delta x} = \frac{e\Delta k}{2\pi}$$

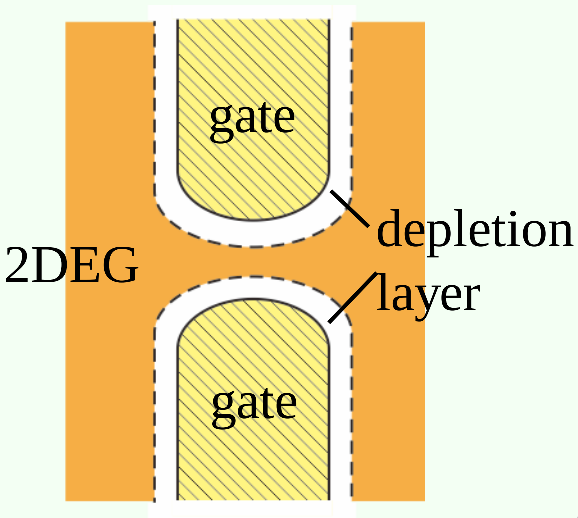
$$J = \frac{e}{\Delta x}\frac{\Delta E}{\hbar \Delta k} = \frac{e^2}{h}V$$

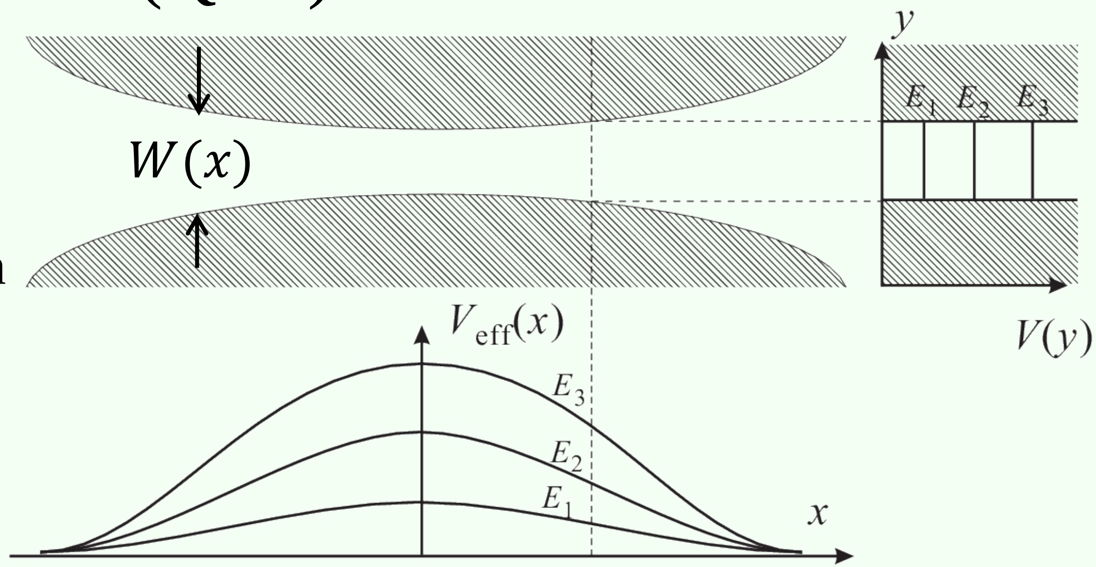
Energy width: $\Delta E = eV$ Wave packet width in time: $\Delta t = \dfrac{h}{\Delta E} = \dfrac{h}{eV}$

$$J = \frac{e}{\Delta t} = \frac{e^2}{h}V$$

Conductance quantum comes from fermion statistics of electrons

Quantum point contact (QPC)



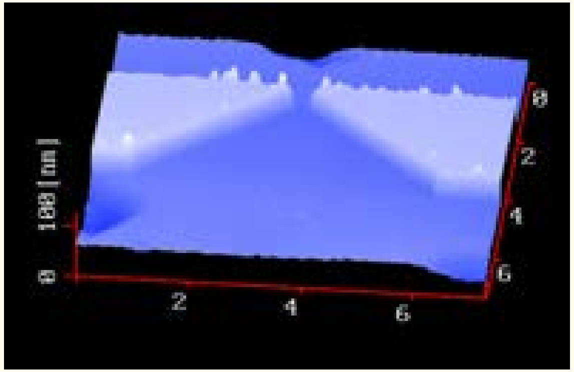


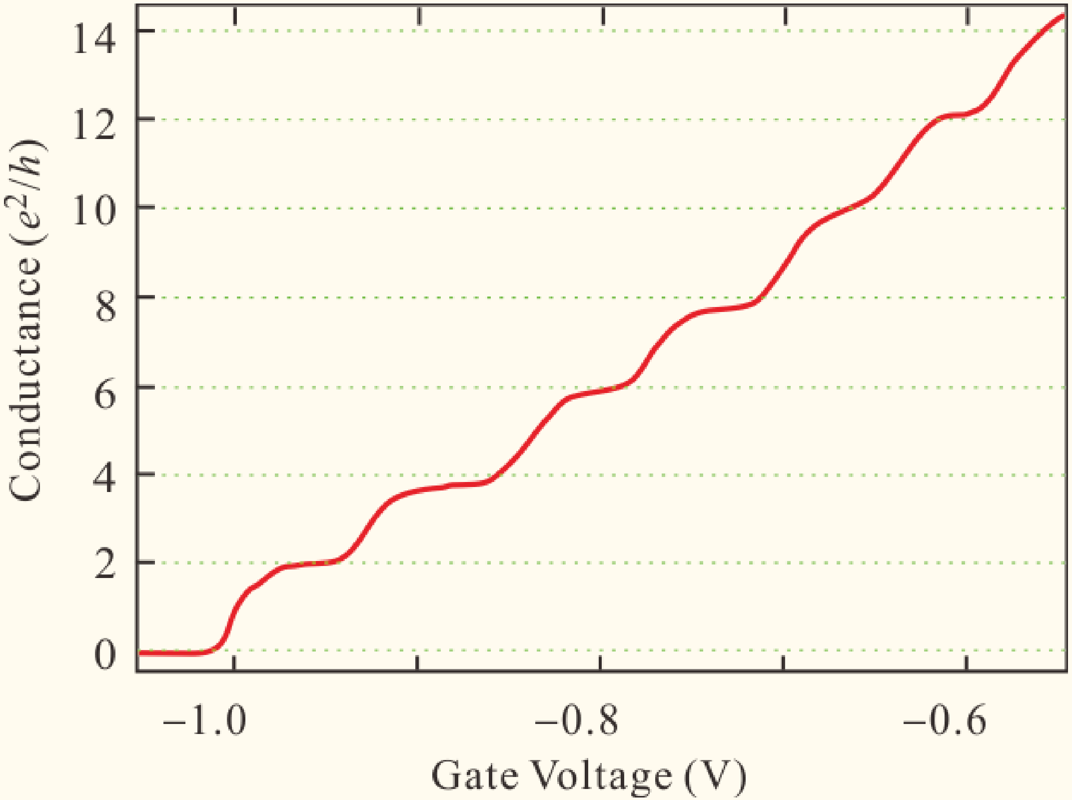
$$H\psi(x,y) = \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\varphi_n(y)\phi(x)$$

$$= \varphi_n(y)\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \left(\frac{n\pi}{2W}\right)^2\right)\phi(x) = E\varphi_n(y)\phi(x)$$

$$V_{\text{eff}}(n,x) = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2W(x)}\right)^2$$

Conductance channel

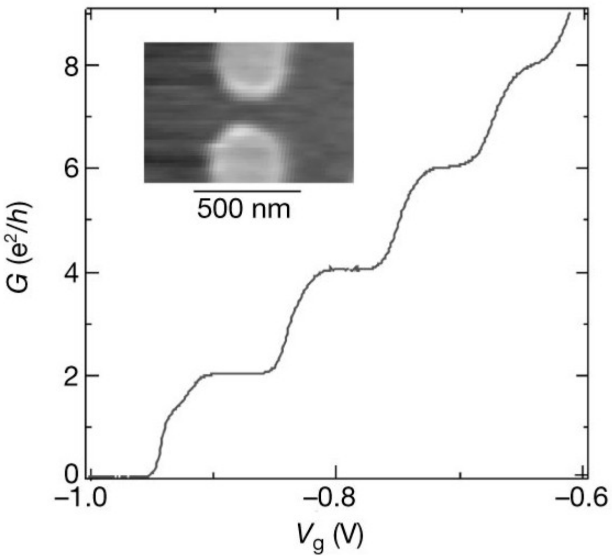


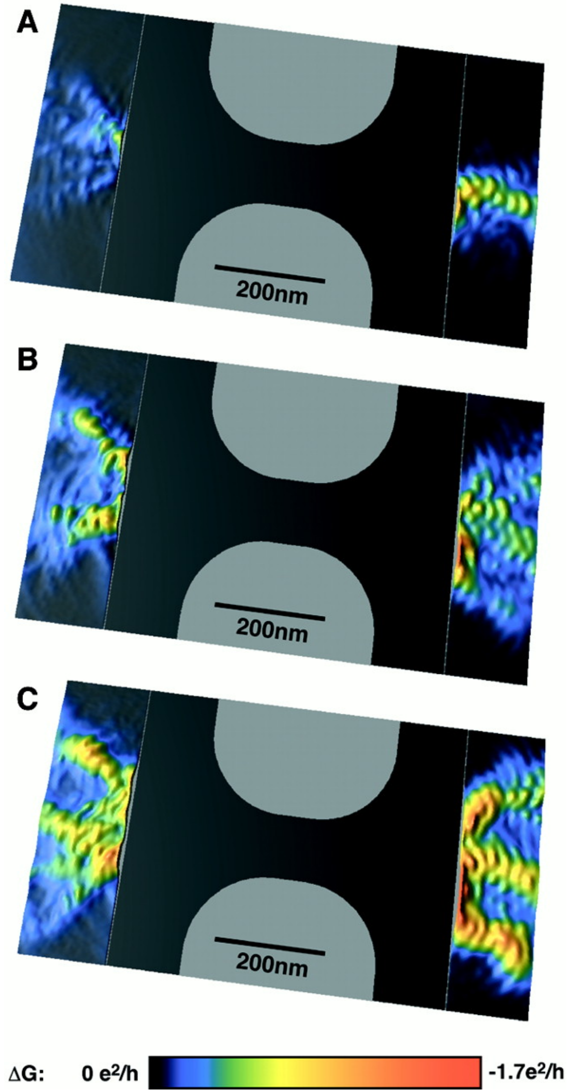


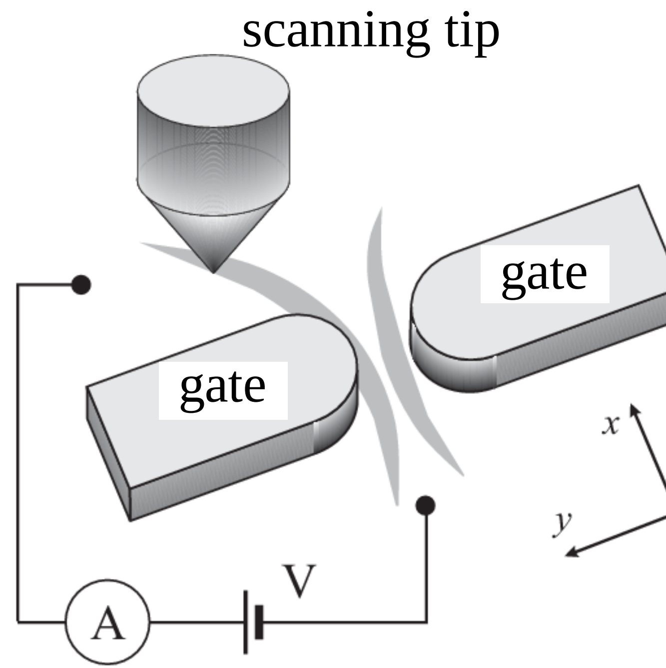
Transmissible one-dimensional system:

Conductance Channel

Scanning tip conductance measurement



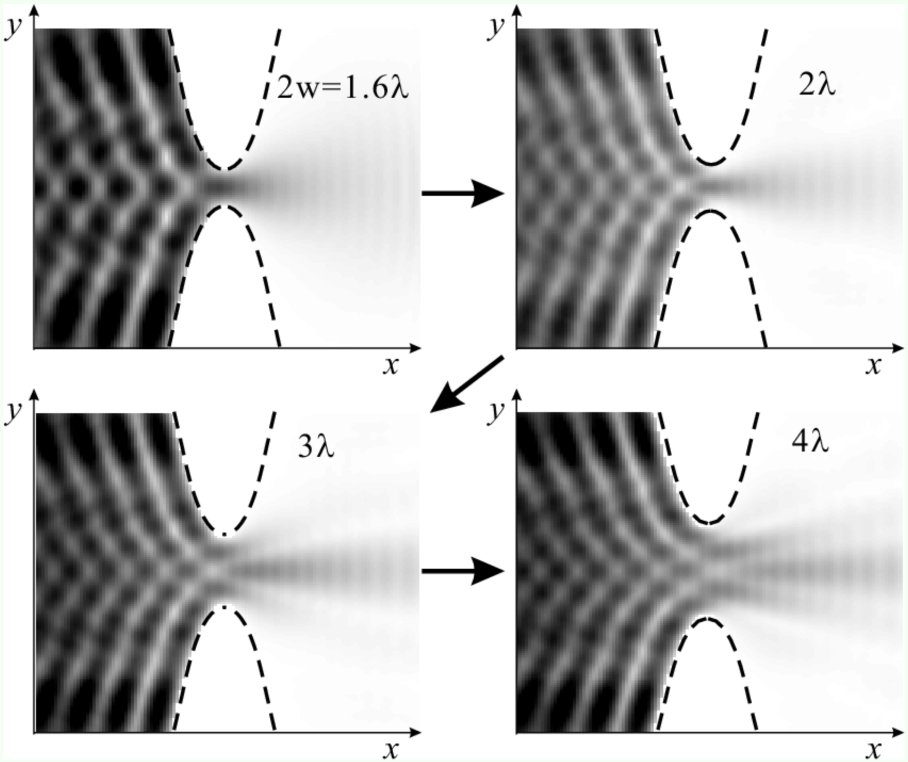




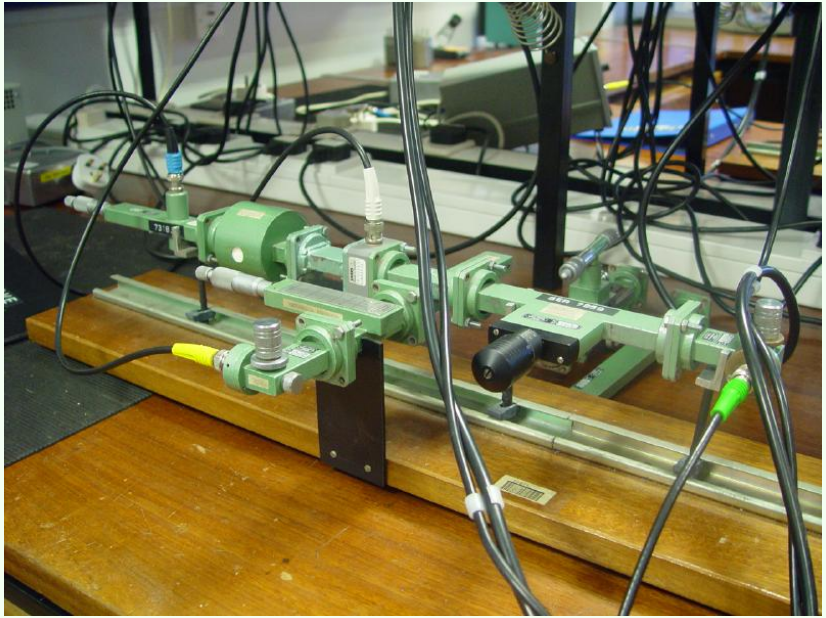
M. A. Topinka et al.,
Nature **410**, 183 (2001)

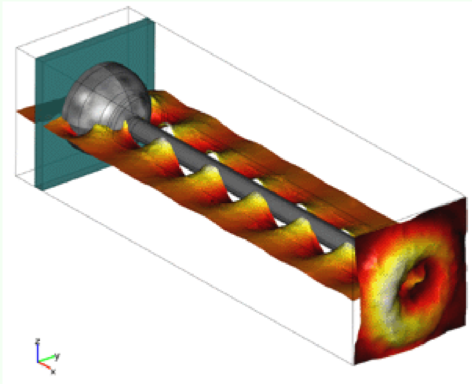
Microwave and electron waveguides

Quantum point contact

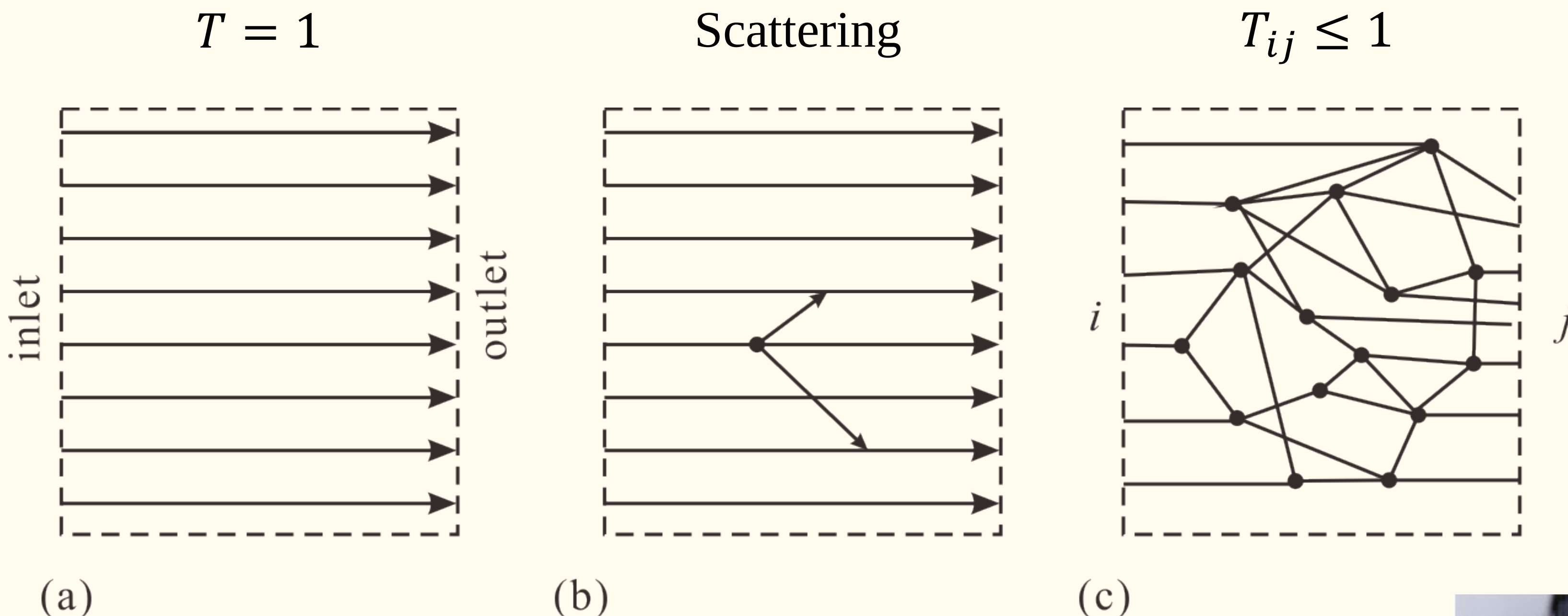


Microwave waveguide





Landauer formula for two-terminal conductance

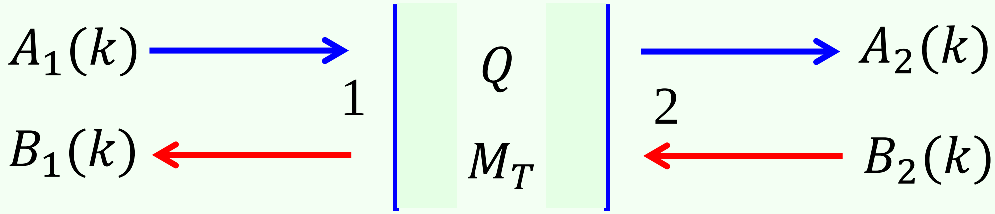


$$G = 2\frac{e^2}{h}\sum_{i,j} T_{ij}$$

Rolf Landauer
1927 - 1999

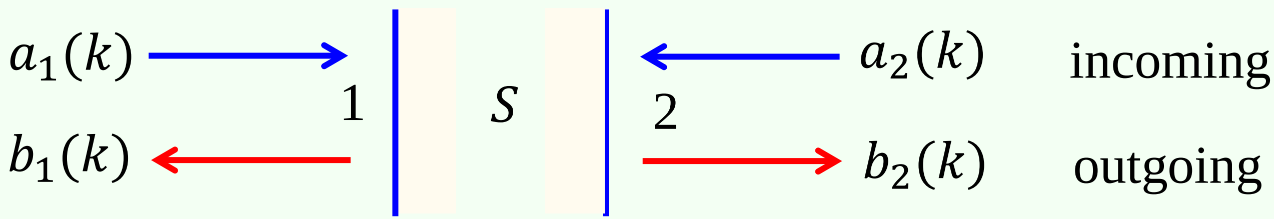
Scattering matrix (S-matrix)

T-matrix



Transfer matrix: M_T $$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \equiv M_T \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

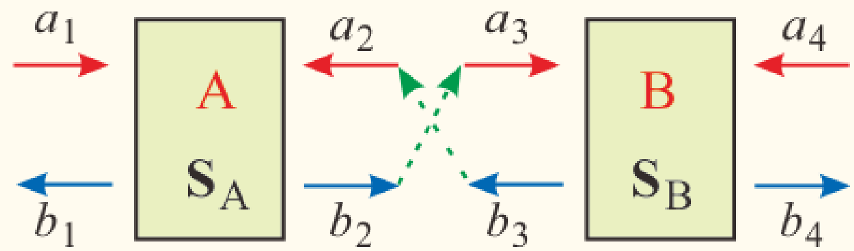
S-matrix



$$\begin{pmatrix} b_1(k) \\ b_2(k) \end{pmatrix} = S \begin{pmatrix} a_1(k) \\ a_2(k) \end{pmatrix} = \begin{pmatrix} r_{\mathrm{L}} & t_{\mathrm{R}} \\ t_{\mathrm{L}} & r_{\mathrm{R}} \end{pmatrix} \begin{pmatrix} a_1(k) \\ a_2(k) \end{pmatrix}$$

Complex probability density flux $$a_i(k) = \sqrt{v_{\mathrm{Fi}}}\,\psi_{ai}(k_{\mathrm{F}})$$

Connection of S-matrix



$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = S_A \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} r_\mathrm{L}^{(\mathrm{A})} & t_\mathrm{R}^{(\mathrm{A})} \\ t_\mathrm{L}^{(\mathrm{A})} & r_\mathrm{R}^{(\mathrm{A})} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix},$$

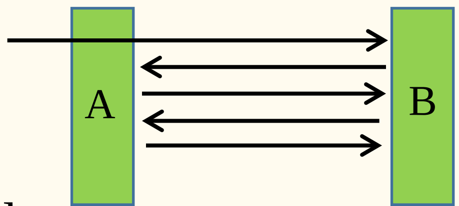
$$\begin{pmatrix} b_3 \\ b_4 \end{pmatrix} = S_B \begin{pmatrix} a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} r_\mathrm{L}^{(\mathrm{B})} & t_\mathrm{R}^{(\mathrm{B})} \\ t_\mathrm{L}^{(\mathrm{B})} & r_\mathrm{R}^{(\mathrm{B})} \end{pmatrix} \begin{pmatrix} a_3 \\ a_4 \end{pmatrix}$$

$$b_2 = a_3, \quad a_2 = b_3$$

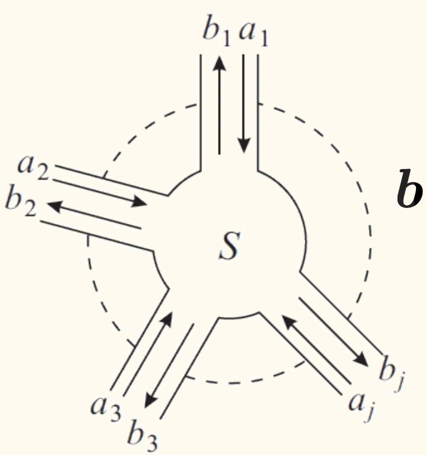
$$S_\mathrm{AB} = \begin{pmatrix} r_\mathrm{L}^{(\mathrm{A})} + t_\mathrm{R}^{(\mathrm{A})} r_\mathrm{L}^{(\mathrm{B})} \left(I - r_\mathrm{R}^{(\mathrm{A})} r_\mathrm{L}^{(\mathrm{B})}\right)^{-1} t_\mathrm{L}^{(\mathrm{A})} & t_\mathrm{R}^{(\mathrm{A})} \left(I - r_\mathrm{L}^{(\mathrm{B})} r_\mathrm{R}^{(\mathrm{A})}\right)^{-1} t_\mathrm{R}^{(\mathrm{B})} \\ t_\mathrm{L}^{(\mathrm{B})} \left(I - r_\mathrm{R}^{(\mathrm{A})} r_\mathrm{L}^{(\mathrm{B})}\right)^{-1} t_\mathrm{L}^{(\mathrm{A})} & r_\mathrm{R}^{(\mathrm{B})} + t_\mathrm{L}^{(\mathrm{B})} \left(I - r_\mathrm{R}^{(\mathrm{A})} r_\mathrm{L}^{(\mathrm{B})}\right)^{-1} r_\mathrm{R}^{(\mathrm{A})} t_\mathrm{R}^{(\mathrm{B})} \end{pmatrix}$$

S-matrix

$$\left(I - r_{\mathrm{R}}^{(\mathrm{A})} r_{\mathrm{L}}^{(\mathrm{B})}\right)^{-1} = I + r_{\mathrm{R}}^{(\mathrm{A})} r_{\mathrm{L}}^{(\mathrm{B})} + \left(r_{\mathrm{R}}^{(\mathrm{A})} r_{\mathrm{L}}^{(\mathrm{B})}\right)^{2} + \left(r_{\mathrm{R}}^{(\mathrm{A})} r_{\mathrm{L}}^{(\mathrm{B})}\right)^{3} + \cdots$$



Multi-channel



$$\boldsymbol{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_i \\ \vdots \\ b_n \end{pmatrix} = \begin{pmatrix} S_{11} & \cdots & S_{1i} & \cdots & S_{1n} \\ \vdots & \ddots & & & \vdots \\ S_{i1} & & S_{ii} & & S_{in} \\ \vdots & & & \ddots & \vdots \\ S_{n1} & \cdots & S_{ni} & \cdots & S_{nn} \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_i \\ \vdots \\ a_n \end{pmatrix} = \mathrm{S}\boldsymbol{a}$$

Reciprocity $S_{ij} = S_{ji}$

(time-reversal symmetry)

Unitarity $\sum_j S_{ji} S_{jk}^{*} = \delta_{ik}$

Onsager reciprocity

Lars Onsager
1903-1976

$$\left[\frac{(i\hbar\nabla + e\boldsymbol{A})^2}{2m} + V\right]\psi = E\psi$$ Complex conjugate and $\boldsymbol{A} \to -\boldsymbol{A}$

$$\left[\frac{(i\hbar\nabla + e\boldsymbol{A})^2}{2m} + V\right]\psi^* = E\psi^*$$ $\{\psi^*(-B)\} = \{\psi(B)\}$

Scattering solution: $\mathrm{Sc}\{a \to b\}$ $\mathrm{Sc}\{\boldsymbol{a}(B) \to \boldsymbol{b}(B)\} \in \{\psi(B)\},\quad i.e.,\quad \boldsymbol{b}(B) = S(B)\boldsymbol{a}(B)$

$$\boldsymbol{b}^*(B) = S^*(B)\boldsymbol{a}^*(B)$$

$$\mathrm{Sc}\{\boldsymbol{b}^*(-B) \to \boldsymbol{a}^*(-B)\} \in \{\psi^*(-B)\} = \{\psi(B)\}\quad i.e.\quad \boldsymbol{a}^*(-B) = S(B)\boldsymbol{b}^*(-B)$$

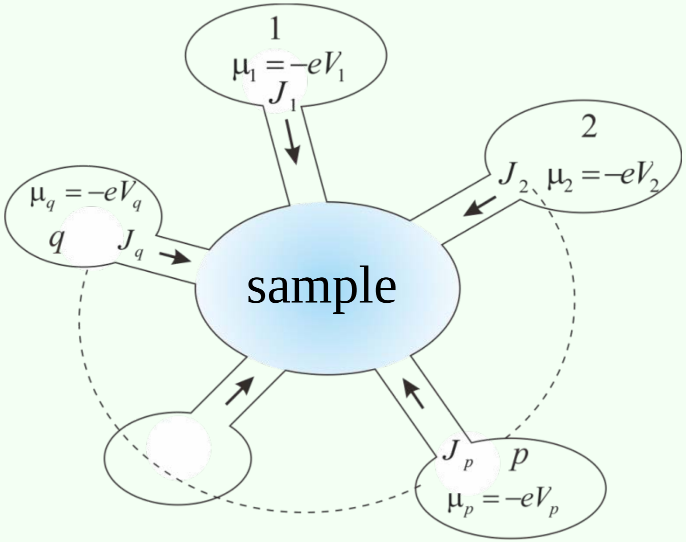
$$\boldsymbol{b}^*(B) = S^{-1}(-B)\boldsymbol{a}^*(B)$$

$$S^*(B) = S^{-1}(-B) = S^\dagger(-B)\ \left(\ \text{unitarity}\ \ SS^\dagger = S^\dagger S = I\right)$$

$$S(B) = {}^tS(-B) \qquad S_{ij}(B) = S_{ji}(-B)$$

Landauer-Büttiker formula

Makus Büttiker
1950-2013



$$J_p = -\frac{2e}{h}\sum_q [T_{q\leftarrow p}\mu_p - T_{p\leftarrow q}\mu_q]$$

$$\mathscr{T}_{pq} \equiv T_{p\leftarrow q}\ \ (p \neq q), \qquad \mathscr{T}_{pp} \equiv -\sum_{q\neq p} T_{q\leftarrow p}$$

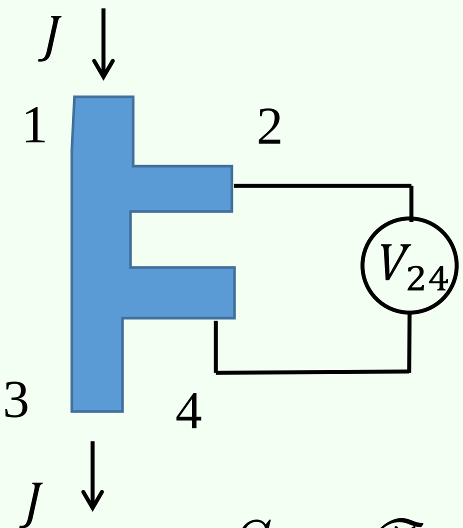
$$\boldsymbol{J} = {}^t(J_1, J_2, \cdots), \boldsymbol{\mu} = {}^t(\mu_1, \mu_2, \cdots)$$

$$\boldsymbol{J} = \frac{2e}{h}\mathscr{T}\boldsymbol{\mu}$$

$$V_q = \frac{\mu_q}{-e}, \qquad G_{pq} \equiv \frac{2e^2}{h}T_{p\leftarrow q}\ \text{ then }\ J_p = \sum_q [G_{qp}V_p - G_{pq}V_q]$$

$$\sum_q J_q = 0 \qquad \sum_q [G_{qp} - G_{pq}] = 0 \qquad G_{qp}(B) = G_{pq}(-B)$$

Landauer-Büttker formula



$$\alpha_{11} = 2G_q[-\mathscr{T}_{11} - S^{-1}(\mathscr{T}_{14} + \mathscr{T}_{12})(\mathscr{T}_{41} + \mathscr{T}_{21})]$$

$$\alpha_{12} = 2G_q S^{-1}(\mathscr{T}_{12}\mathscr{T}_{34} - \mathscr{T}_{14}\mathscr{T}_{32})$$

$$\alpha_{21} = 2G_q S^{-1}(\mathscr{T}_{21}\mathscr{T}_{43} - \mathscr{T}_{23}\mathscr{T}_{41})$$

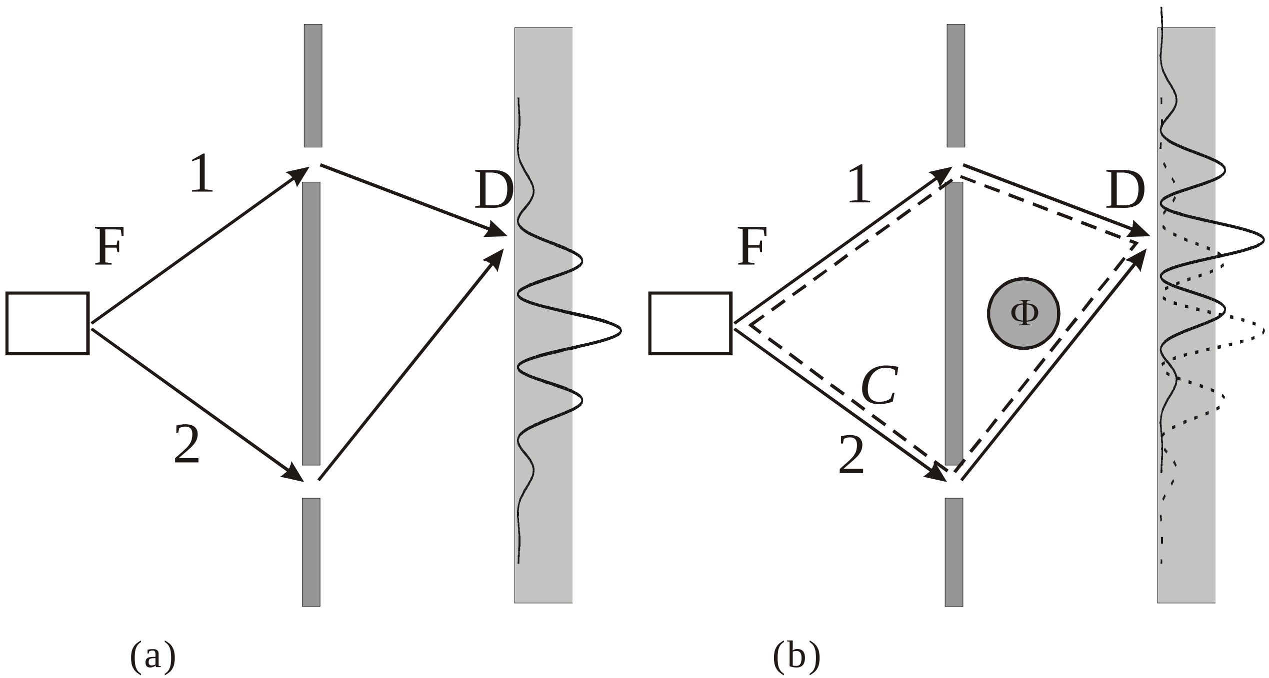
$$\alpha_{22} = 2G_q[-\mathscr{T}_{22} - S^{-1}(\mathscr{T}_{21} - \mathscr{T}_{23})(\mathscr{T}_{32} + \mathscr{T}_{12})]$$

$$S = \mathscr{T}_{12} + \mathscr{T}_{14} + \mathscr{T}_{32} + \mathscr{T}_{34} = \mathscr{T}_{21} + \mathscr{T}_{41} + \mathscr{T}_{23} + \mathscr{T}_{43}$$

$$\mathcal{R}_{13,24} = \frac{V_2 - V_4}{J_1} = \frac{\alpha_{21}}{\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21}}$$

$$\mathcal{R}_{mn,kl}(B) = -\mathcal{R}_{kl,mn}(-B)$$

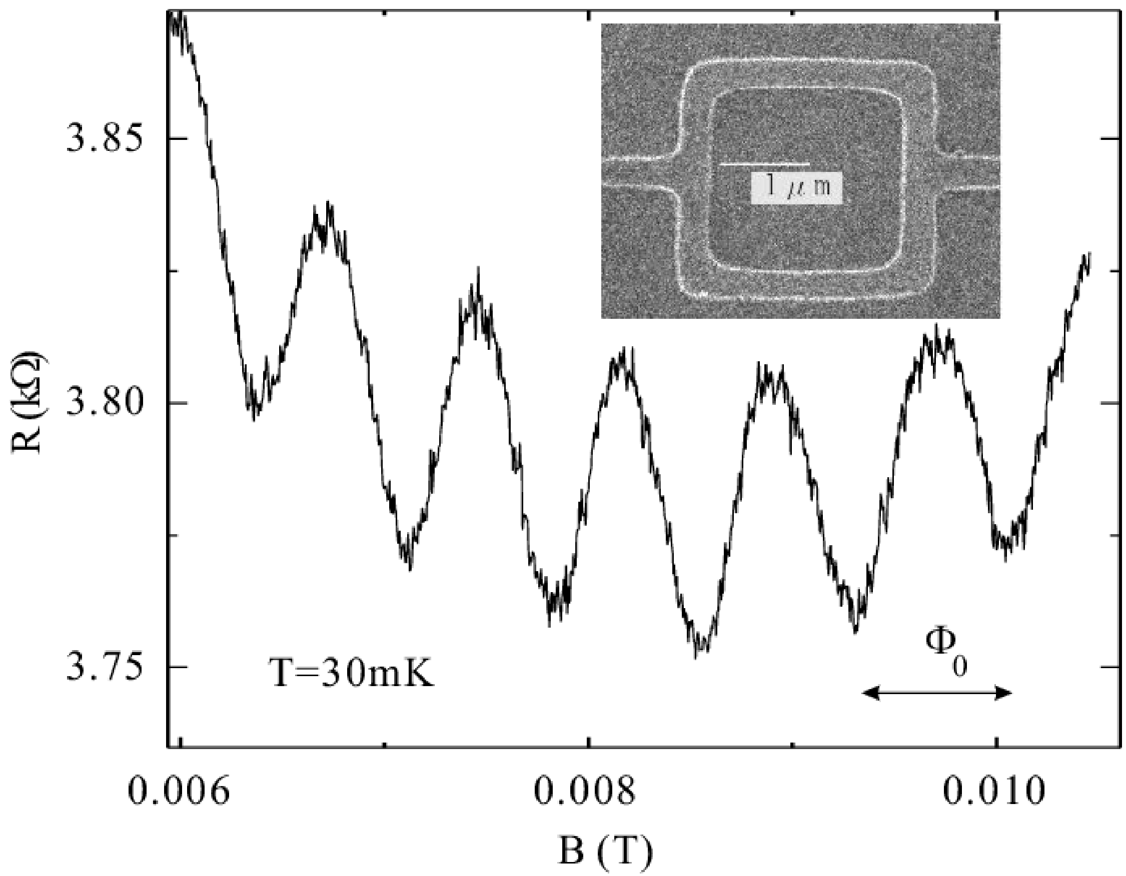
Aharonov-Bohm effect



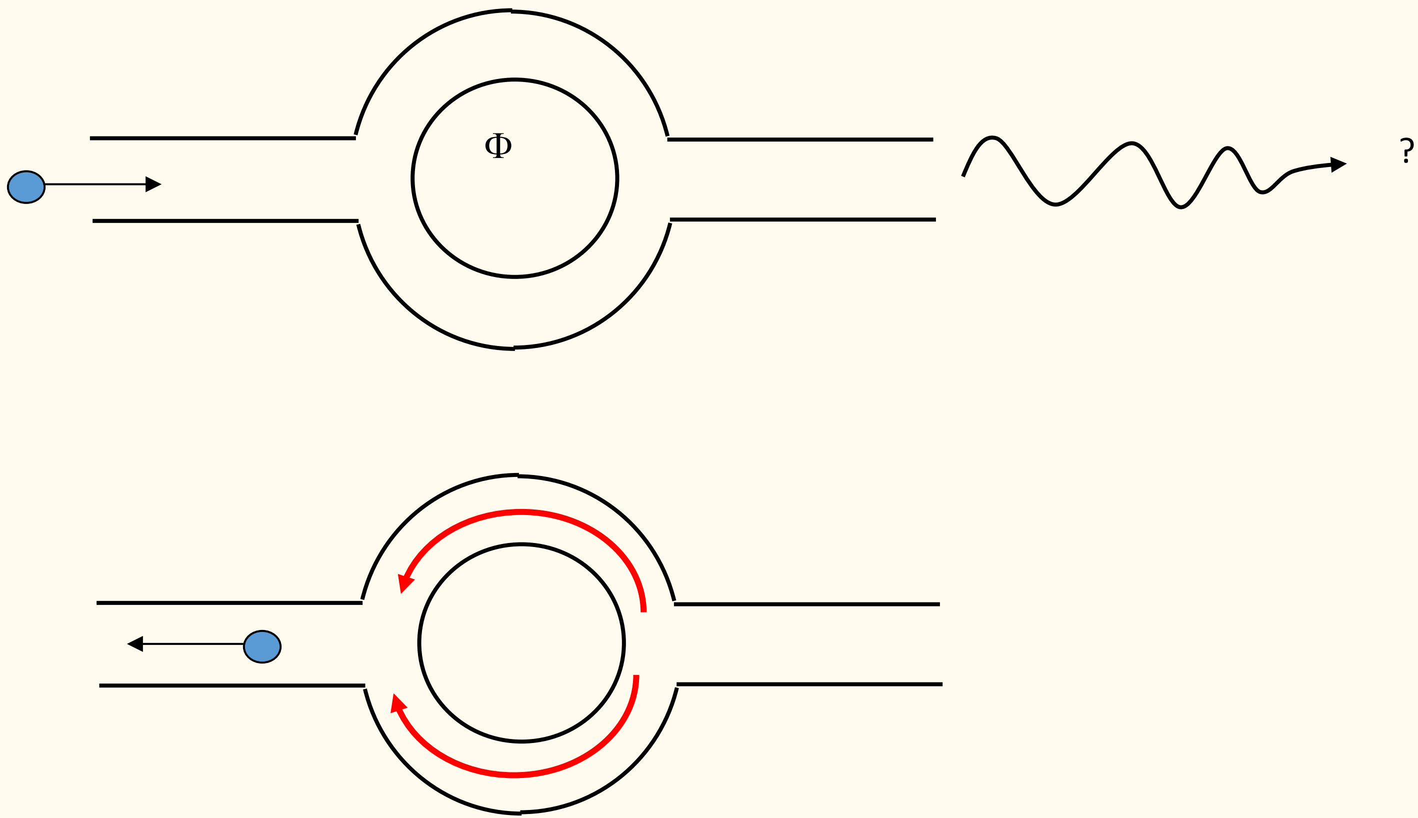
$$\boldsymbol{p} = m\boldsymbol{v} + e\boldsymbol{A} \qquad p = \hbar k = \frac{h}{\lambda}$$

$$\Delta\theta = \frac{e}{\hbar}\oint_C \Delta\boldsymbol{A}\cdot \mathrm{d}\boldsymbol{s} = \frac{e}{\hbar}\int_S \boldsymbol{B}\cdot \mathrm{d}\boldsymbol{n} = 2\pi\frac{\Phi}{\Phi_0} \qquad \Phi_0 \equiv \frac{h}{e}$$

Aharonov-Bohm ring



Disappearance of electrons

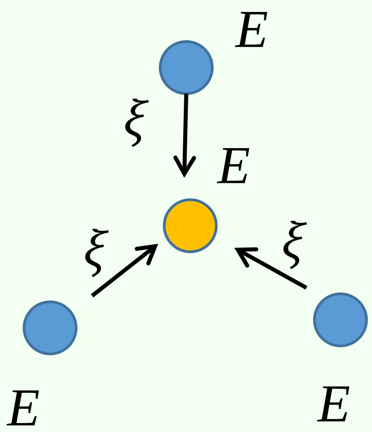


Exercise C-6-20

Energy gap opening in one-dimensional lattice can be easily understood by solving 2x2 Schrodinger equation:

$$i\hbar\frac{\partial}{\partial t}\boldsymbol{a} = \begin{pmatrix} E & \xi \\ \xi & E \end{pmatrix}\boldsymbol{a}$$

which gives eigenvalues $E \pm \xi$



For systematic treatment, the space group theory is the best method to consider this kind of symmetry.
But in the case of graphene, a simple consideration similar to the above is enough to understand why we the off-diagonal terms in Hamiltonian leave degeneracy.
Consider the case illustrated in the left figure and calculate the eigenvalues. Write a brief comment why the degeneracy is not lifted.