Electrons as scattered waves

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Electrons as plane waves

Electron in vacuum is a plane wave

\[
\psi_k(\vec{r}, t) = \frac{1}{\sqrt{V}} \exp(i\vec{k}\cdot\vec{r} - iE(k)t / \hbar)
\]

- \(\psi_k(\vec{r}, t)\) - wavefunction
- \(|\psi_k(\vec{r}, t)|^2\) - probability
- \(V\) - norm. volume
- \(\vec{k}\) - wavevector
- \(\vec{p} = \vec{k}\hbar\) - momentum
- \(E = \frac{(\vec{k}\hbar)^2}{2m}\) - energy
Electrons as fermions

<table>
<thead>
<tr>
<th>Pauli principle:</th>
<th>Number of states in a small cube near ( k )</th>
<th>Fraction of filled states in the cube: filling factor ( f )</th>
</tr>
</thead>
</table>
| A state is either filled or empty | \[
\frac{2_s}{(2\pi)^3} V \sum d k_x d k_y d k_z \] | 

\[
\rho(E) = \int d^3 k \frac{1}{(2\pi)^3} \begin{bmatrix} E(k) \\ \bar{v}(k) \end{bmatrix} f(k) 
\]

\[
\text{current density } \begin{bmatrix} \rho \\ E \end{bmatrix} = \int d^3 k \frac{d^3 k}{(2\pi)^3} \begin{bmatrix} 1 \\ E(k) \end{bmatrix} f(k) 
\]

q.mech. does not set \( f \), statistics does

\[
f_{eq}(k) = f_F(E(k) - \mu)) = \frac{1}{1 + \exp \frac{E - \mu}{k_B T}} 
\]

Zero T: sharp step
Waveguide

1d motion: \( y, z \) – restricted: mode index \( n \), \( x \)- free: \( k_x \)

\[
\psi_{k_x,n}(x, y, z) = \Phi_n(y, z) \exp(ik_x x)
\]

\[
\Phi_n(y, z) \exp(ik_x x)
\]

Standing wave
Plane wave

\[
E_n(k_x) = \frac{(\hbar k_x)^2}{2m} + E_n; \quad E_n = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_y^2}{a^2} + \frac{n_z^2}{b^2} \right)
\]

Dictionary: mode = transport channel
Potential barrier

Intersect the waveguide with a potential barrier $U(x)$

\[ \frac{(\hbar k)^2}{2m} = E; \quad \frac{(\hbar \kappa)^2}{2m} = E - U_0 \]

4 unknown variables: $A, B, r, t$

4 equations:

- continuity of wavefunction and its derivative at two boundaries

Dictionary: reflection and transmission amplitudes
Potential barrier: transmission probability

Result for a rectangular barrier

\[ T(E) \equiv |t|^2 = \frac{1}{1 + \left( \frac{\sin \kappa d (k^2 - \kappa^2)}{2k\kappa} \right)^2} \]

Dictionary: transmission probability, coefficient
Nanostructure versus waveguide

**Nanostructure**: can be very complex

**Can be modelled as**: waveguide with transport channels + potential barrier

**Essence**: set of transmissions $T_n$

Enough to describe the transport!

**To see this**: consider

*Adiabatic Quantum Transport, Quantum Point Contact*
Adiabatic Quantum Transport

Constriction as a potential barrier

\[ E_n(x) = \frac{\pi^2}{2m} \left( \frac{n_y^2}{a^2(x)} + \frac{n_y^2}{b^2(x)} \right) \]

Closed Channels (T=0)

Open Channels (T=1)
Current in a QPC

Filling factors are brought from the reservoirs

\[ I = \frac{2s}{2\pi\hbar} \sum_{n:\text{open}} \int dE \left[ f_L(E) - f_R(E) \right] = \frac{2s}{2\pi\hbar} N_{\text{open}} (\mu_L - \mu_R) = G_Q N_{\text{open}} V \]

\[ N_{\text{att}}(t) = N_{\text{open}} \frac{2s e Vt}{2\pi\hbar} \]

Quantized conductance
Experiment

Van Wees et al. 1988 – experimental evidence of conductance quantization

![Graph showing conductance vs. gate voltage with quantization steps]

Infinitely many transport channels –
Few open channels

Quantization not ideal
Building a Landauer conductor

Adiabatic Quantum Transport

I

II

Quantum Point Contact

Real life

III

QPC with scattering

IV
Scattering matrix

\[ \begin{align*}
N_R + N_L & \quad \text{Incoming amplitudes } \vec{a} \\
N_R + N_L & \quad \text{Outgoing amplitudes } \vec{b}
\end{align*} \]

\[ \vec{b} = \hat{s} \vec{a} \]

\[ \begin{bmatrix} \vec{b}_L \\ \vec{b}_R \end{bmatrix} = \begin{bmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{bmatrix} \begin{bmatrix} \vec{a}_L \\ \vec{a}_R \end{bmatrix} \]

\[ \begin{cases} r_{12} & \\
r_{22} & \\
l & \\
r_{32} & \\
\vdots & \\
\end{cases} \]

\[ \left\{ \begin{array}{c}
t_{12} \\
t_{22} \\
t_{32} \\
\vdots \\
\end{array} \right\} \]
Scattering matrix: properties and example

\[ \hat{s}^+ \hat{s} = \hat{1} \]

unitarity

\[ \hat{t} = \hat{t}' \]

Time reversibility

\[ \hat{r}^+ \hat{r} + \hat{t}^+ \hat{t} = \hat{1} \]

One-channel scatterer

\[ \begin{bmatrix} b_L \\ b_R \end{bmatrix} = \begin{bmatrix} r & t' \\ t & r' \end{bmatrix} \begin{bmatrix} a_L \\ a_R \end{bmatrix} \]

\[ r = \sqrt{\text{Re}^i\theta}; r' = -\sqrt{\text{Re}^{i(2\eta-\theta)}}; \]

\[ t = \sqrt{T e^{i\eta}}; T = 1 - R \]
Landauer formula

Hermitian matrix $\hat{t} + \hat{t}^\dagger$ has a set of eigenvalues $T_p$ at each energy $E$.

The current reads:

$$I = G_Q \sum_p \int dE \, T_p(E) \left( f_L(E) - f_R(E) \right)$$

$$I = G_Q \sum_p T_p \, V$$
Simple-minded derivation

One channel:

Reservoir biased at voltage $V$ sends

$$N_{\text{att}}(t) = \frac{2s eVt}{2\pi\hbar}$$

electrons

Chance to pass: $T_0$

Charge passed: $Q = e T_0 N_{\text{att}}$

Average current:

$$I = \frac{Q}{t} = G_Q T_0 V$$

Many channels: sum over channels

$$I = G_Q \sum_p T_p V$$
Restrictions and limitations

**Restrictions:**
- Elastic scattering: electrons pass without energy loss
- Electrons do not interact (*the same?*)

**Limitations:**
- Nature is generally merciful
- Electrons do not interact close to Fermi level
- Low temperature, voltage are good
- Short structures are good
- Limitations depend on quantity of interest
Counting electrons

How to count correctly?

How to count electrons?
Characteristic function

\[ \Lambda_t(\chi) = \sum_{N} \exp(i\chi N)P_t(N) \]

- Independent events: \( \Lambda \) factorizes
- Time property: \[ \ln \Lambda_t(\chi) \propto t \]
- Elementary event analysis

\[ \ln \Lambda_t(\chi) = t \ln(1+W_1(\exp(i\chi)-1)+W_2(\exp(i2\chi)-1)+...+W_M(\exp(iM\chi)-1)) \]
Two limits

Tunnel junction: $T_n \ll 1$: rare=independent electron transfers

$$
\Lambda_t(\chi) = \exp(\tilde{N}(e^{i\chi} - 1)); \quad \tilde{N} \equiv t < I > / e
$$

QPC: $T_n = 1$: electrons are waves: current does not fluctuate

$$
\Lambda_t(\chi) = \exp(i\chi\tilde{N}); \quad \tilde{N} \equiv t < I > / e
$$
Levitov formula

\[
\ln \Lambda(\chi) = 2_s \Delta t \int \frac{dE}{2\pi\hbar} \sum_p \ln \left\{ 1 + T_p(e^{i\chi} - 1)f_L(1 - f_R) + T_p(e^{-i\chi} - 1)f_R(1 - f_L) \right\}
\]

**Electron transfers**

- Independent in different energy strip
- Independent in different channels
- To the left and to the right: are dependent!
- Transfers at negative energy are blocked!

**Simple example:** electrons transferred in one direction
Electrons gambling

\[ \ln \Lambda(\chi) = N_{at} \ln \left\{ 1 + T_0 (e^{i\chi} - 1) \right\} \]

\[ N_{at} = \frac{2 s e V t}{2 \pi \hbar} \]

- \( N_{at} \) = number of game slots
- \( T_0 \) = winning chance
- \( N \) = number of games won

\[ P_N = \binom{N_{at}}{N} T_0^N (1 - T_0)^{N_{at} - N} \]
Transmission distribution

Person $\rightarrow$ pin-code $\leftarrow$ ATM machine
Quantum Contact $\rightarrow$ $T_p$ $\leftarrow$ Quantum Transport

$\rho(T) = \left\langle \sum_p \delta(T - T_p) \right\rangle$

Diffusive contact:

$\rho(T) = \frac{2\langle G \rangle}{G_Q} \frac{1}{T\sqrt{1-T}}$
Types of quantum contacts

Quantum contact: an individuality: pin-code $T_p$
Type of a quantum contact:= shape of transmission distribution

- Tunnel junction: $T_p \approx 0$
- Realistic QPC $T_p \approx 1$