Today:

- Scattering matrices
  - Combining coherently, + interpretation
  - Combining incoherently
- Landauer-Buttiker in action
  - Experimentally finding the transmission coefficients
  - Another approach (metal contacts)
  - Scattering matrices in nanotubes

Recall our definition of $S$ matrix

\[
\begin{pmatrix}
  B \\ F
\end{pmatrix} = \begin{pmatrix}
  S_{11} & S_{12} \\ S_{21} & S_{22}
\end{pmatrix} \begin{pmatrix}
  A \\ G
\end{pmatrix}
\]

- Unitary matrix that connects incoming and outgoing amplitudes.
- May be rewritten as:

\[
\begin{pmatrix}
  B \\ F
\end{pmatrix} = \begin{pmatrix}
  r & t^* \\ t & r^*
\end{pmatrix} \begin{pmatrix}
  A \\ G
\end{pmatrix}
\]

where $T_{ik}(E) = |S_{2i}|^2$, $R_{ik}(E) = |S_{ii}|^2$
Combining $S$ matrices

What about coherently coupled systems, like this:

$$
\begin{pmatrix}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} & \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
s(1) & s(2)
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
a_5 \\
b_5
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} & \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix}
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} & \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
s(1) & s(2)
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
a_5 \\
b_5
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} & \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix}
\end{pmatrix}
\end{pmatrix}
$$

- Each subsystem in isolation is described by its own scattering matrix, $s^{(0)}$.
- For coherent combination, the composite $s$ matrix =

$$
S = s^{(1)} \otimes s^{(2)}
$$

Combining $S$ matrices

$$
\begin{pmatrix}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} & \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
s(1) & s(2)
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
a_5 \\
b_5
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} & \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix}
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} & \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
s(1) & s(2)
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
a_5 \\
b_5
\end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} & \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix}
\end{pmatrix}
\end{pmatrix}
$$

Use shorthand when writing terms to do with leads (1,3) and (2,4):

$$
\begin{pmatrix}
b_3 \\
b_5
\end{pmatrix} = \begin{pmatrix}
r^{(1)} & t^{(1)} \\
t^{(1)} & r^{(1)}
\end{pmatrix} \begin{pmatrix}
a_3 \\
a_5
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
b_3 \\
b_5
\end{pmatrix} = \begin{pmatrix}
r^{(2)} & t^{(2)} \\
t^{(2)} & r^{(2)}
\end{pmatrix} \begin{pmatrix}
a_3 \\
a_5
\end{pmatrix}
$$

Result:

$$
t = t^{(1)} [ I - r^{(1)} r^{(2)} ]^{-1} t^{(1)}
\Rightarrow
r = r^{(1)} + t^{(1)} [ I - r^{(1)} r^{(2)} ]^{-1} t^{(1)}
\Rightarrow
r' = r^{(2)} + t^{(2)} [ I - r^{(1)} r^{(2)} ]^{-1} r^{(1)} t^{(2)}
\Rightarrow
t' = t^{(1)} [ I - r^{(2)} r^{(1)} ]^{-1} t^{(2)}
$$
Interpretation of result: Feynman paths

\[ t = t^{(2)} [I - r^{(1)} r^{(2)}]^{-1} t^{(1)} \]
\[ r = r^{(1)} + t^{(1)} r^{(2)} [I - r^{(1)} r^{(2)}]^{-1} t^{(1)} \]

\[ t' = t^{(1)} [I - r^{(2)} r^{(1)}]^{-1} t^{(2)} \]
\[ r' = r^{(2)} + t^{(2)} [I - r^{(1)} r^{(2)}]^{-1} r^{(1)} r^{(2)} \]

Take first equation and expand:

\[ t = t^{(2)} [I - r^{(1)} r^{(2)}]^{-1} t^{(1)} \]
\[ = t^{(2)} t^{(1)} + t^{(2)} [r^{(1)} r^{(2)}] t^{(1)} + t^{(2)} [r^{(1)} r^{(2)} ][r^{(1)} r^{(2)}] t^{(1)} + \ldots \]

Direct product of S matrices equivalent to summing over all possible Feynman paths - assumes complete coherence.

Combining S matrices incoherently

As you might guess, incoherent combination means instead of combining S matrices (adding amplitudes), we combine probability matrices (adding probabilities).

\[ \begin{pmatrix} r^{(1)} \\ t^{(1)} \end{pmatrix} \quad \begin{pmatrix} r^{(2)} \\ t^{(2)} \end{pmatrix} \quad \text{dephasing} \quad \begin{pmatrix} r^{(2)} \\ t^{(2)} \end{pmatrix} \]

\[ P^{(1)} \equiv \begin{pmatrix} \left| \psi^{(1)} \right|^2 \\ \left| \psi^{(1)} \right|^2 \end{pmatrix} \equiv \begin{pmatrix} R^{(1)} \\ T^{(1)} \end{pmatrix} \]

Result from combining two probability matrices:

\[ T = \frac{T^{(1)} T^{(2)}}{1 - R^{(1)} R^{(2)}} \]

Note: no oscillatory piece in denominator - loss of interference effects.
Partial coherence

How to do this? One method: add extra fictitious leads.

\[
\begin{pmatrix}
  r^{(1)} & t^{(1)} \\
  t^{(1)} & r^{(1)}
\end{pmatrix}
\quad \quad \quad 
\begin{pmatrix}
  r^{(2)} & t^{(2)} \\
  t^{(2)} & r^{(2)}
\end{pmatrix}
\]

- Have some amplitude for scattering into these leads (where dephasing then occurs), and some amplitude for emission from these leads, such that no net current flows.
- By tuning those amplitudes, can tune from fully coherent to fully incoherent extremes.

Take-home message: Landauer-Buttiker approach + scattering matrix formalism lets us model quantum coherent systems well.

Landauer-Buttiker in action

Two basic uses of LB formalism:

- Use theory to calculate \( T(E) \), and try to predict / retrodict measured transport characteristics.
- From experimental data, try to infer \( T(E) \) or \( S \), and use that to understand physical system in question - check for consistency or other physics.

First approach frequently used in molecular electronics experiments - will see later.
We’ll look at second approach today in 3 systems.
Cross geometry

Shephard et al., PRB 46, 9648 (1992).

• Usual GaAs 2deg + Au gates.
• Can imagine trying to infer transmission coefficients by fixing chemical potentials for various leads, and measuring appropriate currents.

How to measure $T_{pq}$

• Fix chemical potential of 3 leads and measure currents into / out of them.
• Fix current into 4th lead and measure chemical potential there.

\[
\begin{pmatrix}
I_1 \\
I_2 \\
I_3 \\
I_4
\end{pmatrix} =
\begin{pmatrix}
T_{11} & T_{12} & T_{13} & T_{14} \\
T_{21} & T_{22} & T_{23} & T_{24} \\
T_{31} & T_{32} & T_{33} & T_{34} \\
T_{41} & T_{42} & T_{43} & T_{44}
\end{pmatrix}
\begin{pmatrix}
\mu_1 \\
\mu_2 \\
\mu_3 \\
\mu_4
\end{pmatrix} = \begin{pmatrix}
\mu_1 \\
0 \\
0 \\
-\mu_4
\end{pmatrix}
\]

\[
T_{\text{eff}} = \frac{h}{2e \mu_i} (i \neq 1)
\]

\[
(T_{11} - M_4) = \frac{h}{2e \mu_i}
\]
Using those coefficients for a prediction

So, by cycling around the 4 leads, can infer all 16 matrix elements.

Knowing these, can we predict anything? Yes!

\[
\begin{align*}
\bar{T}_F &= \bar{T}_{13} = \bar{T}_{31} = \bar{T}_{24} = \bar{T}_{42} \\
\bar{T}_R &= \bar{T}_{21} = \bar{T}_{32} = \bar{T}_{43} = \bar{T}_{14} \\
\bar{T}_L &= \bar{T}_{12} = \bar{T}_{23} = \bar{T}_{34} = \bar{T}_{41}
\end{align*}
\]

With these definitions, can predict the Hall resistance, assuming we know \(T\)s as function of magnetic field.

\[
R_H = \frac{h}{2e^2} \frac{T_R^2 - T_L^2}{(T_R + T_L)[T_R^2 + T_L^2 + 2T_R(T_R + T_L)]}
\]

Using those coefficients for a prediction

Does this actually work?

Can measure transmission coefficients for various values of magnetic field and different gate voltages….
Using these coefficients for a prediction

Solid line = prediction based on measured $T$s.
Dashed line = measured values for Hall resistance.
Small variations b/c gate voltages must be cycled back and forth from 0 between measurements of the $T$s and the Hall measurement.

This is a great example of a 4 terminal device where measuring the transmission coefficients allows predictions of complicated behaviors without knowing details of, e.g., disorder in the sample.

Scattering matrices and nanotubes


Metallic single-walled carbon nanotube between two very good contacts.
Observation: differential conductance near zero bias oscillates as a function of gate voltage.

Basic idea: 1d Fabry-Perot interference! Changing $V_G$ varies $k_F$, and thus the number of electron wavelengths fitting between contacts.

Slight complication: 2 1d subbands, each with slightly different $k$ values when $V_G$ is nonzero.
Scattering matrices and nanotubes

\[
\begin{align*}
S_T & = S_L \times S_R \\
S_N & = S_L \times S_N \times S_R \\
S_N & = S_N \times S_R \\
S_T & = S_T \times S_R
\end{align*}
\]
Scattering matrices and nanotubes

By modeling scattering matrices (estimating reflectances of interfaces) and gate coupling (how much $k_F$ changes with $V_G$), can predict modulation of conductance with bias and gate voltage very well.

Metal-metal junctions: another method of inferring $T$

• Already saw that clean atomic-scale metal junctions can show conductance quantization.
• Not obvious that one atom = one channel with $T \sim 1$.
• In particular, metals with complicated band structures could have contributions from many different orbitals ($p$, $d$).
• Result: $G$ vs. $t$ while breaking can be messy.

Subgap structure

- In superconducting junctions, it’s possible to use “subgap structure” (basically tunneling conductance for $eV < $ energy gap) to figure out how many channels, and $T_i$ for each channel.

![Graph showing current vs. voltage for different configurations](image)

Example: Pb junction in 5 different configurations. Can fit data very well by assuming 4 channels contribute to $G$ rather than just 1.

Role of chemical structure here

Upshot: in clean atomic-scale metal junctions, one can use superconductivity to infer number of channels and transmission coefficients for each channel.

Chemical structure of the constituent atoms dominate these properties!

Example: even when $G \approx 2e^2/h$ in Al junction, turns out that’s from 3 channels (one for each $p$ orbital!) each with a transmission coefficient of around 1/3 - can be modeled through quantum chemistry calculations.
Summary:

- Landauer-Buttiker picture actually does work in real experiments.
- It is possible to experimentally determine relevant quantities (transmission coefficients, scattering matrices) and use these to determine whether overall physics is understood in real devices.
- *Origins* of those transmission coefficients, etc., are often rooted in the microscopic details of the device under examination.

Next time:

- Next up: transistors - a primer; + demands of the electronics industry.