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

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

$$
T_{LR}(E) = |S_{21}|^2 \\
T_{RL}(E) = |S_{12}|^2 \\
R_{LR}(E) = |S_{11}|^2 \\
R_{RL}(E) = |S_{22}|^2
$$

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

$$
\begin{pmatrix}
B \\
F
\end{pmatrix} = \begin{bmatrix}
r & t' \\
t & r'
\end{bmatrix} \begin{pmatrix}
A \\
G
\end{pmatrix}
$$

where \( T_{LR}(E) = |t|^2 \), etc.
Combining $S$ matrices

What about coherently coupled systems, like this:

- Each subsystem in isolation is described by its own scattering matrix, $s^{(j)}$.
- For coherent combination, the composite $s$ matrix =
  $$S = S^{(1)} \otimes S^{(2)}$$
Combining $S$ matrices

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

$$
\begin{pmatrix}
  b_{13} \\
  b_{5}
\end{pmatrix} =
\begin{pmatrix}
  r^{(1)} & t^{(1)} \\
  t^{(1)} & r^{(1)}
\end{pmatrix}
\begin{pmatrix}
  a_{13} \\
  a_{5}
\end{pmatrix}
\quad
\begin{pmatrix}
  a_{5} \\
  b_{24}
\end{pmatrix} =
\begin{pmatrix}
  r^{(2)} & t^{(2)} \\
  t^{(2)} & r^{(2)}
\end{pmatrix}
\begin{pmatrix}
  b_{5} \\
  a_{24}
\end{pmatrix}
$$

Result:

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

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

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

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

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

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

Take first equation and expand:

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

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

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

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

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

dehasing

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

\[
\begin{pmatrix}
    r^{(1)} & t^{n(1)} \\
    t^{(1)} & r^{n(1)} \\
\end{pmatrix} \rightarrow \mathbf{P}^{(1)} \equiv \begin{pmatrix} |r^{(1)}|^2 & |t^{n(1)}|^2 \\ |t^{(1)}|^2 & |r^{n(1)}|^2 \end{pmatrix} = \begin{pmatrix} R^{(1)} & T^{(1)} \\ T^{(1)} & R^{(1)} \end{pmatrix}
\]

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.

- 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

- 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.

$$\frac{h}{2e} \begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_4 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{21} & T_{31} & T_{41} \\ T_{12} & T_{22} & T_{32} & T_{42} \\ T_{13} & T_{23} & T_{33} & T_{43} \\ T_{14} & T_{24} & T_{34} & T_{44} \end{pmatrix} \begin{pmatrix} \mu_1 \\ 0 \\ 0 \\ 0 \end{pmatrix} - M_1 \begin{pmatrix} \mu_1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$T_{q1} = \frac{h}{2e} \frac{I_q}{\mu_1} \quad (i \neq 1)$$

$$(T_{11} - M_1) = \frac{h}{2e} \frac{I_1}{\mu_1}$$
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!

\[ T_F \equiv T_{13} = T_{31} = T_{24} = T_{42} \]
\[ T_R \equiv T_{21} = T_{32} = T_{43} = T_{14} \]
\[ T_L \equiv T_{12} = T_{23} = T_{34} = T_{41} \]

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

\[ R_H = \frac{h}{2e^2} \frac{T_R^2 - T_L^2}{(T_R + T_L)[T_R^2 + T_L^2 + 2T_F(T_F + T_R + T_L)]} \]
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
Scattering matrices and nanotubes
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 $eV < \text{energy gap}$) to figure out how many channels, and $T_i$ for each channel.

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 $G \sim 2e^2/h$ 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.