Electronic Properties of Nanoparticles and Nanostructures

- Semiconductor Nanodevices
  - Lithographically defined quantum dots
- Nanowires
- Metal nanoparticles
- Carbon Nanotubes
- Single Molecules
**Nano-Physics**

What makes nanostructures different?

- **Classical Effects:** "Coulomb Blockade"
  - Single-electron charging energy may be greater than $k_BT$.

- **Quantum Effects**:
  - Discreteness of Energy Levels (Closed System)
  - Quantum Interference Effects on transport properties

  *Examples:*
  - "Quantization" of Conductance through a constriction
  - Quantum Breakdown of the Coulomb Blockade
  - "Universal" Conductance Fluctuations
  - Effects of Magnetic Fields: Aharonov-Bohm Oscillations, Persistent Currents, Magnetoresistance...

  Generally: Low Temperature Effects
Coulomb Charging Energy

Particle: Coupled capacitively to Gate + to Ground Plane.
Coupled by weak tunnel junctions to Source & Drain.

Charging energy \( E_c = \frac{(Q - \overline{Q})^2}{2C} + \text{const.} \)

- \( Q = \text{charge on particle (electrons - protons)} = Ne \)
  with \( N = \text{integer} \)
- \( \overline{Q} = V_g \cdot C_g, \) varies continuously with \( V_g \)
- \( C_g = \text{capacitance between particle & gate} \)
- \( C = \text{total capacitance of dot} \)

Let \( U = \frac{e^2}{2C} = \text{"charging energy"} \)

\( \overline{Q} = \frac{\overline{Q}}{e} \)
**SET:** Single Electron Transistor

Assume: $U \gg k_B T$

$V_{\text{drain}} = -\frac{V}{2}$, $V_{\text{source}} = \frac{V}{2}$, $V \ll U$

Conduction Occurs by 2-Step Tunneling Process:

1. Electron Below Fermi Level of Source Tunnels onto Particle ($N \rightarrow N+1$)

2. Electron from particle goes into empty state above Fermi Level of Drain ($N+1 \rightarrow N$)

Energy must be conserved at each step if tunneling matrix elements are small.

Must have $|U| \ll 2x1 < 1 eV$; i.e., for small $U$.

Sharp maximum in conductance at $x = \frac{1}{2}$:

$$i_e \approx V_g \approx (n + \frac{1}{2}) \frac{e}{C_g}$$

(arbitrary integer $n$)
\[ E_c = U (N - \bar{N})^2 \quad : \quad \bar{N} = \text{continuous parameter} \times V_g \]

Minimum energy shown by \textbf{Blue} curve:

Periodic in \( V_g \) : \( N = \text{closest integer to \( \bar{N} \) :} \)

- If \( \bar{N} = \frac{N + \alpha}{1} \) with \( -\frac{1}{2} \leq \alpha < \frac{1}{2} \), \( n = \text{integer} \):
  \[ E_c^{\text{min}} = U \alpha^2 \quad , \quad N = n \]
  \[ E(N+1) - E(N) = U (1 - 2\alpha) \geq 0 \]
  \[ E(N+1) - E(N) = 0 \iff \alpha = \frac{1}{2} \]

Typically: \( U \) is large compared to energy spacing \( \delta \) between single electron quantum levels:

\[ S \approx E_F / \text{Molecules} \sim E_F / R^3 \]

\[ U \approx \frac{e^2}{\varepsilon R} \text{ for isolated sphere of radius } R \]

or \( U \approx \frac{e^2 d}{\varepsilon A} \) when \( d = \text{thickness of dielectric layer} \) \( (\text{Plane Capacitors}) \)
The **SINGLE-ELECTRON TRANSISTOR**

**Coulomb Blockade**

**Conductance Peaks**

\[ G = \frac{dI}{dV} \quad (V \rightarrow 0) \]

Classical Model:

- Peaks equally spaced.
- Finite width due to \( T \neq 0 \).
Note: If "tunneling rates" between particle and either source or drain are sufficiently great — it is not necessary to conserve energy in intermediate state: extra electron spends only short time on particle, can be "off energy shell."

Then get quantum mechanical breakdown of Coulomb Blockade Effect.
Effect of Discrete Energy Levels

Constant Interaction Model

Energy of Dot: \( E = U(N - \bar{N})^2 + \sum_{j=1}^{N} E_j \)

\( E_j = j^{th} \) single-particle energy level

- Energy to Add \( N^{th} \) Electron:
  \( E(N) - E(N-1) = \varepsilon_N + 2U \cdot (N - \bar{N} - \frac{1}{2}) \)

\( N^{th} \) Electron Enters when \( E(N) - E(N-1) = 0 \),

or \( \bar{N} = \bar{N}_N = (N - \frac{1}{2}) + \frac{\varepsilon_N}{2U} \)

- Spacing Between Successive Conductance Peaks:

\( \bar{N}_{N+1} - \bar{N}_N = 1 + \frac{\varepsilon_{N+1} - \varepsilon_N}{2U} \)

- Measures spacing between successive energy levels
Level Spacing:

Non-interacting Electrons, \( B = 0^+ \):
- Fill levels alternately, spin up, spin down.

\[ E_{N+1} - E_N \] should be zero if \( N \) is odd;
\[ E_{N+1} - E_N \] should be \( > 0 \) if \( N \) is even, with

distribution given by "Random Matrix Theory" (Wigner-Dyson)

\[ P(\Delta E) \]

\( \delta \)-function with weight \( \frac{1}{2} \)

\( \Delta \) = "mean level spacing"

"Bi-modal"
Effects of Electron-Electron Interactions and Fluctuation Effects

Example: For even number of electrons, if $E_{n+1} - E_n$ is small compared to mean level spacing $\Delta$, then Exchange Interaction may make it favorable to put one electron in state $n$ and one in state $n+1$, with total spin $S = 1$, rather than two electrons in level $N$ with $S = 0$.

Then levels are not filled with alternating spin up, spin down.

Distribution of Coulomb Peak Spacings is altered.

Even if successive electrons go into the same electron level, there is an energy cost due to exchange, which is typically comparable to a fraction of $\Delta$.

Distribution typically no-longer bimodal.
Statistics of Coulomb Blockade

Peak Spacings (in a GaAs quantum dot). Results of C.M. Marcus & coworkers (SR Patel et al PRL 1998)

CI + SDRMT = Constant Interaction Model with Spin-Degenerate Single Particle Energies distributed according to "Random Matrix Theory" (Wigner Dyson)
Effects of Finite Coupling to Leads

LARGE Coupling: Coulomb blockade peaks completely disappear. Number of electrons on dot are no longer quantized. No longer have discrete energy levels on dot. Quantum interference effects at low temperatures give rise to "fluctuations" in the conductance as a function of gate voltage, applied magnetic field, other parameters.

Large Coupling $\Leftrightarrow G > \frac{2e^2}{h} = 80\mu\text{s}$
**Intermediate Coupling To Leads**

(Temperature << Separation between single particle energy levels)

- Coulomb Blockade Peaks Acquire Width due to Coupling

- Conductance values in Valleys increase, with difference between with EVEN or ODD number of electrons on dot.

In ODD case Valley can disappear (for T\to0) due to "Kondo Effect"
Kondo Effect in a Single-Walled Carbon Nanotube
Experiments by Liang, Bockrath, and Park
"Quantization" of conductance through a narrow constriction.

Quantum Transport in Semiconductor Nanostructures 111

Fig. 44. Point contact conductance as a function of gate voltage at 0.6 K, demonstrating the conductance quantization in units of $2e^2/h$. The data are obtained from the two-terminal resistance after subtraction of a background resistance. The constriction width increases with increasing voltage on the gate (see inset). Taken from B. J. van Wees et al., Phys. Rev. Lett. 60, 848 (1988).

GaAs

$$\frac{2e^2}{h} \approx \frac{1}{13,000 \Omega} \approx 80 \mu s$$
Quantum Mechanics: Narrow Channel

Increasing negative voltage on gates, (on surface) repels electrons in 2D Electron Gas.

Can narrow or pinch off conducting region.

Self-consistent confining potential $V(x, y)$.

Assume rapidly varying function of $y$ and slowly varying function of $x$.

First solve for quantum states of electron motion in y direction as fixed $x$:

Energies $E_n, x$

Wave functions: $f_{n, x}(y)$

$n = 1, 2, 3, \ldots$
Then: make "adiabatic approximation"

\[ y'(x,y) = \phi(x) \cdot \delta_n(x,y) \]

\( \phi \) obeys:

\[ \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U_n(x) \right] \phi(x) = E \phi(x) \]

\[ U_n(x) = V(x, y=0) + E_{n,x} \quad \text{Confinement energy in } y \text{ direction.} \]

= Effective potential for electron in transverse mode \( n \).

Assume: \( U_n(x) \) has a parabolic maximum at \( x=0 \)

Neglect possible scattering between modes

Compute transmission probability

\[ T_n(E) \text{ for a particle in mode } n, \text{ incident at energy } E: \]

\[ T_n \sim \frac{1}{1 + e^{-\frac{(E-U_n(0))}{\hbar \omega}}} \]

For wide barrier: \( \omega_0 \to 0 \),

\[ T_n \sim \Theta(E-U_n(0)) \quad \text{(Step function)} \]
What happens if you have several constrictions in series?

(Low Temperatures, No inelastic Scattering: Resistances do not add.)

If perfectly adiabatic, \( G = \frac{2e^2}{h} N_{\text{min}} \)

\( N_{\text{min}} = \# \text{ of channels in narrowest neck.} \)

If rough, even if \( E \) scattering in region between constrictions, "anything can happen" depending on phase differences: interference effects.
2. Terminal Conductance: Landauer Formula.

\[ G = 2 \frac{e^2}{h} \sum_n T_n \]

\[ T_n = \frac{\text{Transmission}}{\text{Probability for the } n^{th} \text{ Channel}} \]

\[ \frac{e^2}{h} = \frac{1}{26,000 \Omega} \approx 40 \mu S \]

For adiabatic junctions:
\[ T_n \text{ is either 1 or 0.} \]

\[ G = 2 \frac{e^2}{h} \times \text{Number of Open Channels} \]
REFERENCES FOR THE LECTURE OF B. I. HALPERIN


