Quantum Transport in Electron Devices and Novel Materials

ECE 5390/MSE 5472
Fall, 2015

Debdeep Jena (djena@nd.edu)
ECE & MSE, Cornell University
Outline

Part I: Review of fundamentals
1. Review of classical and quantum mechanics
2. Current flow in quantum mechanics
3. Quantum statistics, quest for equilibrium as the driver for transport

Part II: Single-particle transport
4. Ballistic transport: Quantized conductance, Ballistic MOSFETs
5. Transmission and tunneling, Tunneling FETs
6. Closed vs. open systems, the Non-Equilibrium Green’s Function approach to transport
7. Diffusive transport: Boltzmann transport equation, scattering, electron-phonon interactions
8. High-field effects, Gunn diodes and oscillators for high-frequency power

Part III: Many-particle correlated transport
9. Fock-space way of thinking transport, second quantization, conductance anomalies
10. BCS theory of superconductivity, Josephson junctions
11. Landau/Ginzburg theories of phase transitions due to broken symmetry

Part III: Geometrical and topological quantum mechanics, unification with relativity
12. Spin, transport in a magnetic field, Quantum Hall effect, Berry phase in quantum mech
13. Chern numbers, Edge/Topological states, Topological insulators and Majorana Fermions
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About the class

Class website: https://courses.cit.cornell.edu/ece5390/2015_ece5390.htm

ECE 5390 / MSE 5472: Quantum Transport in Electron Devices and Novel Materials
Fall 2015, Cornell University

Instructor
Prof. Debdeep Jena (djena@cornell.edu), Cornell University
Departments of ECE and MSE, Cornell University
Office(s): Bard 326, Phillips 415

Class Hours
MW 8:40 – 9:55 am
Location: Snee Hall 1120, Official Link
Office hours: TBD

Prerequisites
Quantum mechanics, and ECE 4070 (or an equivalent course in solid-state physics).

About the course
Modern electronic and photonic devices are increasingly incorporating new materials with a richer set of underlying physical phenomena in transport that are not covered in traditional materials and device courses. A deep understanding of the underlying physics is key to controlling, and designing devices based on transport and electrostatics. This course first connects the traditional “continuum” transport physics of micron-scale devices, to coherent quantum transport in nanoscale devices, and shows the major technical bottlenecks device physicists and engineers face in the coming decades. By rigorously developing emergent topological and correlated ideas in quantum transport, the course will arm students with tools that will be used to invent new devices in the future.

Topics
The course will cover the fundamentals of charge, heat, and spin transport in semiconductor electron devices and emerging materials such as 2D crystals and correlated oxides. The topics that will be covered are:
- Electronic gain and bandwidth, and its link to transport.
- Boltzmann transport equation, scattering, Fermi’s golden rule, defect scattering, and electron-phonon interactions.
- Transport coefficients, thermoelectric properties. Mobility, high-field saturation and impact ionization.
- Analogies of high-field transport to phenomena in high-energy physics.
- Gunn and IMPATT devices, ultrafast (THz) semiconductor electronics.
- Tunneling transport, backward diodes, negative differential resistance.
- Coherent transport in semiconductors, ballistic transport, quantized conductance.
- The non-equilibrium Green’s function method, contacts as integral to devices.
- Metal-insulator transitions, Landau-Ginzburg models for phase transitions due to broken symmetry.
- Correlated transport in BCS superconductivity in semiconductors such as diamond and MoS2.
- Magnetotransport, quantum Hall effects, the Berry phase and Chern numbers.
- Edge-state/surface transport phenomena in emerging chiral semiconductors.
- Topological insulators, and symmetry-protected dissipationless transport.

Handouts/Notes
Course calendar [planned]

Assignments
Class website: https://courses.cit.cornell.edu/ece5390/2015_ece5390.htm

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About the class

ECE 5390/MSE 5472 || Cornell University, Fall 2015

Quantum Transport in Electron Devices and Novel Materials

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Topics:
- Electronic gain and bandwidth, and its link to transport.
- Boltzmann transport equation, scattering, Fermi’s golden rule.
- Electron-phonon interactions, mobility, high-field saturation and impact ionization.
- Analogies of high-field transport to phenomena in high-energy physics.
- Gunn and IMPATT devices, ultrafast (THz) semiconductor electronics.
- Tunneling transport, backward diodes, negative differential resistance.
- Coherent and ballistic transport, quantized conductance.
- The non-equilibrium Green’s function method, contacts as integral to devices.
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Website: https://goo.gl/vU94we

Debdeep Jena (djena@cornell.edu), Cornell University
About the class
About the class

Electronic switches today

- Earlier this week (August 11th) Intel announced...
Our goals in this course

- Communication Devices
  - Semiconductor Transistor
  - Vacuum tube

- Logic Devices
  - Digital Switch
  - Mechanical relay

- Quantum limits?
- New Materials with better transport
- Speed (Bandwidth)

- Charge-based
- Spin-based
- Correlated/Phase transitions
Our goals in this course

As engineers, cards we are dealt with:

\[ \text{Si} \rightarrow N \]

Our tasks:

1. Improve (Gain) + (Bandwidth) + better communication
2. Lower energy cost of computation + better 'logic'.

How do we coax electrons and the elements
to do these things for us?

- Learn the physics of transport in materials (semiconductors, metals, etc).
- Learn how to control the electrons' population, spins, etc.
- Learn the 'traditional' or semi-classical transport properties such as drift, diffusion, scattering, etc. Examine limitations on devices.
- Learn 'emergent' phenomena in transport: e.g. Gunn Oscillations, Superconductivity, Quantum Hall effects, etc. Metal-Insulator transitions, etc.
- Learn the most modern tools for coherent quantum transport such as the NEGF approach. Expose its limitations.
- Learn how historically how transport phenomena have led to new device applications.
Maxwell’s equations: Classical EMag

\[ \nabla \cdot \mathbf{D} = \rho, \quad \text{Gauss’s law} \]
\[ \nabla \cdot \mathbf{B} = 0, \quad \text{Gauss’s law} \]
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad \text{Faraday’s law} \]
\[ \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}, \quad \text{Ampere’s law.} \]
Maxwell’s equations: Classical EMag

\[(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2})E = 0, \quad \text{Wave Equations}\]

\[(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2})B = 0.\]

Far Field

**Figure 20.2:** Antenna producing an electromagnetic wave.
Maxwell’s equations: Birth of Light

\[(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) \mathbf{E} = 0, \quad \text{Wave Equations}\]

\[(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) \mathbf{B} = 0.\]

\[
\mathbf{E} = E_0 e^{i(k_z z - \omega t)} \hat{x}
\]

\[
\mathbf{B} = \frac{E_0}{c} e^{i(k_z z - \omega t)} \hat{y}
\]

\[
\mathbf{S} = \frac{E_0^2}{\eta_0} e^{2i(k_z z - \omega t)} \hat{\mathbf{z}}
\]

**Figure 20.3:** Electromagnetic wave.
Maxwell’s equations: Response of solids

\[ F = q(E + v \times B) \]

\[ P = \varepsilon_0 \chi_e E \]

\[ D = \varepsilon_0 E + P \]

\[ B = \mu_0 (H + \chi_m H) = \mu_0 (1 + \chi_m) H = \mu H \]

**Figure 20.4:** Dielectric and Magnetic materials. Orientation of electric and magnetic dipoles by external fields, leading to electric and magnetic susceptibilities.
Time-evolution of a classical ‘charged’ object

\[ F = -\nabla V(r) = \frac{dp}{dt} \]

Path is deterministic

\[ F = q(E + v \times B) \]

Path is deterministic

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Experiment: Light is a wave... or a particle?

"WAVE"

many photons

laser one?

"PARTICLE"

screen with an array of detectors

Intensity!

double slit

Tune down the intensity!

Intensity

Recover this!

keep doing this again + again

only one detector clicks!

"PARTICLE"
Experiment: Light is a wave… or a particle?

- The only way an object of mass $m=0$ can have momentum is if its speed $v=c$, or the speed of light.
- A photon is exactly such an object. No mass, all energy, and a finite momentum!

**Planck's hypothesis for photons to explain expts:**

$$p = \hbar k$$

$$k = (2\pi/\lambda)\hat{n}, \quad \hat{n} \text{ the direction of propagation}$$

$$\omega = c|k| \text{ with } c \text{ the speed of light}$$

$$E = \hbar \omega$$

**Einstein: look downstairs!**

$$p = mv/\sqrt{1 - (v/c)^2}$$
An electron is a particle... or a wave?
An electron is a particle... or a wave?

Electron beam incident on a crystal (RHEED)

Atomic structure of a crystal (grating!)

Electron diffraction pattern on a screen

Guowang Li (Results from our lab!)

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Wave and particle → need for a wavefunction

Quantum states (electrons, photons) behave as waves AND particles. How do we describe them quantitatively?

- The state of the free quantum particle cannot be represented by independent ‘numbers’ $(x, p_x)$.
- We need a function whose amplitude oscillates in space, yet its magnitude never goes to zero.
- The complex exponential $e^{ikx}$ satisfies these requirements, and respects the uncertainty relation.

The complex exponential $e^{i\frac{px}{\hbar}} = e^{ikx}$ oscillates with $x$, yet $|A|^2$ is constant! $\Rightarrow$ good candidate for a wavefunction that respects $\Delta x \Delta p \geq \frac{\hbar}{2}$. 

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Constructing wavefunctions: superposition

By linear superposition of complex exponentials, we can create ‘particle’ like or ‘wave’ like states as desired for the problem.

\[ \psi(x) = \sum_{\alpha} A_{\alpha} e^{\frac{i\alpha x}{\hbar}} \]

Drawing on Fourier series, we realize that we can create any wavefunction shape to capture the correct physics of the problem. Note the corresponding reciprocal space weight distribution.

The best we can do to locate a "particle" is a 'wavepacket'.

\[ A_{\alpha} \left( e^{\frac{i\alpha x}{\hbar}} + \right) \]

is an allowed "wavefunction".

- Drawing on Fourier series, we realize that we can create any wavefunction shape to capture the correct physics of the problem. Note the corresponding reciprocal space weight distribution.
The states of definite value of an operator are called the eigenstates of that operator.

Unlike classical mechanics, some operators fail to commute!

\[ x\hat{p} - \hat{p}x = [x, \hat{p}] = i\hbar. \]

Non-commuting actions...
Ref: Gamow, Thirty years that shook physics.
Definite momentum, and definite location states

A state of definite location $x_0$:
Must be an eigenstate of operator $x$, with eigenvalue $x_0$:

$$x \psi_{x_0}(x) = x_0 \psi_{x_0}(x) \implies \psi_{x_0}(x) = \delta(x - x_0)$$

Definite in real space $\rightarrow$ spread out in momentum

A state of definite momentum $p$:
Must be an eigenstate of operator $-ih(d/dx)$, with eigenvalue $p$:

$$\hat{p}_x \psi_p(x) = p_x \psi_p(x) \implies -i\hbar \frac{d}{dx} \psi_p(x) = p_x \psi_p(x)$$

$$\psi_p(x) = Ae^{i \frac{px}{\hbar}} = Ae^{ikx}$$

Definite in momentum $\rightarrow$ spread out in real space

States of definite location and definite momentum are unique in quantum mechanics.
States of definite energy: Schrödinger equation

States of definite energy are not unique, because they depend on the ‘potential’ $V(x)$

In classical mechanics, the energy of a particle is:

$$E_{cl} = \frac{p^2}{2m} + V(r)$$

In quantum mechanics, $r$ & $p$ cannot be simultaneously determined because $[x,p]=ih$. Thus, we must solve an equation to obtain the energy.

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right] \psi_E(x) = E \psi_E(x).$$

The Schrödinger equation gives us the prescription to find the states of definite energy.

$$\left[\frac{\hat{p}^2}{2m} + V(r)\right] |\psi\rangle = E |\psi\rangle$$
The Postulates of Quantum Mechanics

The five basic postulates of quantum mechanics are:

1. The state of any physical system at a given time $t$ is completely represented by a state vector $|\Psi\rangle = |\Psi(r,t)\rangle$.

2. For an observable quantity $A$ there is an operator $\hat{A}$. The eigenvalues of $\hat{A}$ are the possible results of the measurements of $A$, that is, denoting the eigenvalues of $\hat{A}$ by $a$,

$$\hat{A}|a\rangle = a|a\rangle,$$  \hspace{1cm} (2.23)

and the probability of a measurement of $A$ yielding the value $a$ at time $t$ is $|\langle a|\Psi(t)\rangle|^2$. The $a$’s, which are the results of possible measurements, must be real. This implies that $\hat{A}$ must be a linear hermitian operator.

3. A measurement of $|\Psi\rangle$ that leads to an eigenvalue $a_i$ leads the quantum mechanical system to collapse into the eigenstate $|\Psi_i\rangle$, which is the eigenstate corresponding to the eigenvalue $a_i$. So a measurement affects the state of the quantum system.

4. There exists a hermitian operator $\hat{H}$ such that

$$i\hbar \frac{\partial |\Psi(r,t)\rangle}{\partial t} = \hat{H}|\Psi(r,t)\rangle.$$  \hspace{1cm} (2.24)

5. Two classical dynamical variables $a, b$, which are conjugate in the Hamiltonian sense, are represented by Schrodinger operators $\hat{A}, \hat{B}$, which obey

$$\hat{A}\hat{B}_j - \hat{B}_j\hat{A}_i = i\hbar \delta_{ij}.$$  \hspace{1cm} (2.25)
The free electron

\[ -\frac{\hbar^2}{2m_e} \frac{d^2}{dx^2} \psi(x) = E \psi(x) \]

\[ \psi(x) = Ae^{ikx} + Be^{-ikx} \]

\[ k = \sqrt{\frac{2m_eE}{\hbar^2}} = \frac{2\pi}{\lambda} \]

\[ E = \frac{\hbar^2 k^2}{2m_e} \]

\[ \hat{p}_x \psi(x) = -i\hbar \frac{d}{dx} \psi(x) = -i\hbar(ikAe^{ikx} - ikBe^{-ikx}) = \hbar k(Ae^{ikx} - Be^{-ikx}) \neq p\psi(x) \]

but... for \( \psi_\downarrow(x) = Ae^{ikx} \),

\[ \hat{p}_x \psi_\downarrow(x) = -i\hbar \frac{d}{dx} \psi_\downarrow(x) = -i\hbar(ikAe^{ikx}) = \hbar k\psi_\downarrow(x) = p\psi_\downarrow(x) \]  

\( V(x) = 0 \)

Allowed momenta are continuous

Energy spectrum is continuous

Not a momentum eigenstate

momentum eigenstate

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Restrict particle in space → Quantization

If we restrict the ‘particle’ in one space, it quantizes the allowed ‘vectors’ in the reciprocal space.

\[ \psi_p(x + L) = \psi_p(x) \]  \[ e^{ikL} = 1 = e^{i2\pi \times n}, \text{ and } k_n = n \times (2\pi/L). \text{ Here } n = 0, \pm 1, \pm 2, ... \]

\[ \psi_n(x) = \frac{1}{\sqrt{L}} e^{i k_n x} \]

\[ k_n = \frac{2\pi}{L} n \quad n = 0, \pm 1, \pm 2, \pm 3, ... \]

Call this ‘state vector’ \( |n\rangle \).

The state functions form a ‘set’

\[ \left\{ \cdots, \psi_{-3}(x), \psi_{-2}(x), \psi_{-1}(x), \psi_0(x), \psi_1(x), \psi_2(x), \psi_3(x), \cdots \right\} \]

Note:

\[ \int_{-L}^{L} \psi^*_n(x) \psi_m(x) \, dx = \delta_{nm} \quad \Rightarrow \text{functions are ORTHOGONAL!} \]

\[ \langle n | n \rangle = \delta_{nm} \quad \Rightarrow \text{Vectors are “perpendicular”!} \]

The set of wave functions \([...\psi_{-3}(x), \psi_{-2}(x), \psi_{-1}(x), \psi_0(x), \psi_1(x), \psi_2(x), ...]\) are special. We note that \( \int_0^L dx \psi_{m}(x) \psi_n(x) = \delta_{nm}, i.e., \text{the functions are orthogonal. Any general wavefunction representing the particle } \psi(x) \text{ can be expressed as a linear combination of this set. This is the principle of superposition, and a basic mathematical result from Fourier theory. Thus the quantum mechanical state of a particle may be represented as } \psi(x) = \sum_n A_n \psi_n(x). \text{ Clearly, } A_n = \int dx \psi_n^*(x) \psi(x). \text{ Every wavefunction constructed in this fashion represents a permitted state of the particle, as long as } \sum_n |A_n|^2 = 1. \]

- The set of states \{...|-1>, |0>, |+1>, ...\} is an orthogonal basis for constructing the wavefunction.
- One can draw an analogy to vector spaces, and use the tools of linear algebra on states.

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3.4 Not so free: particle in a ring

The particle on a ring

\[ \psi(x + L) = \psi(x) \rightarrow e^{ik(x+L)} = e^{ikx} \rightarrow e^{ikL} = 1 \rightarrow kL = 2n\pi \]

Momentum is quantized

\[ k_n = \frac{2\pi}{L} n, \quad n = 0, \pm 1, \pm 2, \ldots \]

\[ \psi(n, x) = Ae^{inkx} \]

Particle on a ring

\[ \int_0^L dx |\psi(n, x)|^2 = 1 \rightarrow |A|^2 \times L = 1 \rightarrow A = \frac{1}{\sqrt{L}} \rightarrow \psi(n, x) = \frac{1}{\sqrt{L}} e^{inkx} \]

Note that \( n = 0 \) is allowed as a result of the periodic boundary condition.

Energy spectrum is discrete, Zero energy is allowed

\[ E_n = \frac{\hbar^2 k_n^2}{2m_e} = n^2 \frac{(2\pi\hbar)^2}{2m_e L^2} = n^2 \frac{\hbar^2}{2m_e L^2} \]

Angular momentum is quantized

\[ L = \frac{p \times r = \hbar k_n \times \frac{L}{2\pi} = \frac{2\pi\hbar}{L} n \times \frac{L}{2\pi} = n\hbar} \]
The particle in a box

\[ V(x) = 0, \quad 0 \leq x \leq L \]
\[ V(x) = \infty, \quad x < 0, x > L \]

The major change is that \( \psi(x) = 0 \) in regions where \( V(x) = \infty \).

\[ \psi(x) = Ae^{ikx} + Be^{-ikx} \rightarrow \psi(0) = 0 = A + B, \psi(L) = Ae^{ikL} + Be^{-ikL} = 0 \]

\[ \frac{A}{B} = -e^{-i2kL} = -1 \rightarrow 2kL = 2n\pi \rightarrow k_n = \frac{n\pi}{L}, n = \pm 1, \pm 2, \pm 3, \ldots \]

Note that \( n = 0 \) is not allowed, because then \( \psi(x) = 0 \) and there is no particle wavefunction after normalization over the length \( L \) is

\[ \psi(n, x) = \sqrt{\frac{2}{L}} \sin(n\frac{\pi}{L} x) = \sqrt{\frac{2}{L}} \sin(k_n x) \]

Energy spectrum is discrete, zero energy NOT allowed!

\[ E_n = n^2 \frac{(\pi \hbar)^2}{2m_e L^2} = n^2 \frac{\hbar^2}{8m_e L^2} \]
The harmonic oscillator

Energy levels equally spaced
Zero energy NOT allowed!

\[ V(x) = \frac{1}{2} m_\omega^2 x^2 \]

Harmonic Oscillator

\[ a = \sqrt{\frac{m\omega}{2\hbar}} (\hat{x} + \frac{i}{m\omega} \hat{p}) \]
\[ a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} (\hat{x} - \frac{i}{m\omega} \hat{p}) \]
\[ \hat{x} = \frac{\sqrt{\hbar}}{2m\omega} (a^\dagger + a) \]
\[ \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} (a^\dagger - a) \]

Can solve the problem using raising and lowering operators

The functions \( H_n \) are the Hermite polynomials,

\[ H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2}) \]

The corresponding energy levels are

\[ E_n = \hbar \omega \left( n + \frac{1}{2} \right) \]

Energy levels equally spaced
Zero energy NOT allowed!

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The harmonic oscillator

The creation/annihilation operator formalism will be key in the ‘second quantization’ methods to be developed later in the course!

\[ V(x) = \frac{1}{2} m_\omega^2 x^2 \]

\[ \hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) \]

\[ \hat{p} = i \sqrt{\frac{m\omega\hbar}{2}} (a^\dagger - a) \]

\[ E_n = (n + \frac{1}{2})\hbar\omega \]

\[ a = \sqrt{\frac{m\omega}{2\hbar}} (\hat{x} + \frac{i}{m\omega} \hat{p}) \]

\[ a|n\rangle = \sqrt{n}|n - 1\rangle \]

\[ a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} (\hat{x} - \frac{i}{m\omega} \hat{p}) \]

\[ a^\dagger|n\rangle = \sqrt{n + 1}|n + 1\rangle \]

\[ \hat{n} = a^\dagger a \]

\[ \hat{H} = \hbar\omega (a^\dagger a + \frac{1}{2}) \]
The hydrogen atom

**Energy levels**

The energy levels of hydrogen, including fine structure, are given by the Sommerfeld expression:

\[
E_{jn} = -\frac{m_e c^2}{2 n^2} \left[ 1 + \frac{\alpha}{n - j + \frac{1}{2} + \sqrt{(j + \frac{1}{2})^2 - \alpha^2}} \right]^{-1/2} - 1
\]

where \( \alpha \) is the fine-structure constant and \( j \) is the “total angular momentum” quantum number, which is equal to \( l \pm \frac{1}{2} \) depending on the direction of the electron spin. The factor in square brackets in the last expression is nearly one; the extra term arises from relativistic effects (for details, see #Features going beyond the Schrödinger solution).

The value

\[
\frac{m_e c^2 \alpha^2}{2} = 0.51 \text{ MeV} = 13.6 \text{ eV}
\]

**Wavefunction**

The normalized position wavefunctions, given in spherical coordinates are:

\[
\psi_{n\ell m}(r, \vartheta, \varphi) = \sqrt{\frac{2}{na_0}} \frac{(n - \ell - 1)!}{2n(n + \ell)!} e^{-\rho/2} \rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho) Y_{\ell m}^m(\vartheta, \varphi)
\]

where:

\[
\rho = \frac{2r}{na_0},
\]

\( a_0 \) is the Bohr radius,

\( L_{n-\ell-1}^{2\ell+1}(\rho) \) is a generalized Laguerre polynomial of degree \( n - \ell - 1 \), and

\( Y_{\ell m}^m(\vartheta, \varphi) \) is a spherical harmonic function of degree \( \ell \) and order \( m \). Note that the generalized Laguerre polynomials are defined differently by different authors. The usage here is consistent with the definitions used by Messiah,\(^8\) and Mathematica.\(^9\) In other places, the Laguerre polynomial includes a factor of \( (n + \ell)! \)\(^10\) or the generalized Laguerre polynomial appearing in the hydrogen wave function is \( L_{n+\ell}^{2\ell+1}(\rho) \) instead.\(^11\)

The quantum numbers can take the following values:

\[
n = 1, 2, 3, \ldots
\]

\[
\ell = 0, 1, 2, \ldots, n - 1
\]

\[
m = -\ell, \ldots, \ell.
\]
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The classical Drude model

**Paul Drude (1900)**

\[ m \frac{dv}{dt} = qE - \frac{mv}{\tau} \]

steady state: \( \frac{d}{dt} (...) \to 0 \)

\[ v = \frac{q\tau}{m} E = \mu E \]

\[ J = qnv = \frac{nq^2\tau}{m} E = \sigma E \implies \sigma_0 = \frac{nq^2\tau}{m} \]

**Oscillating field:**

\[ E(t) = E e^{i\omega t} \]

\[ m \frac{dv}{dt} = qE e^{i\omega t} - \frac{mv}{\tau} \]

\[ v(t) = v(0) e^{i\omega t} \]

**ac conductivity**

\[ \sigma(\omega) = \frac{\sigma_0}{1 + i\omega\tau} = \frac{\sigma_0}{1 + (\omega\tau)^2} - i \frac{\omega\tau \sigma_0}{1 + (\omega\tau)^2} \]

\[ \text{Re}(\sigma(\omega)) \quad \text{Im}(\sigma(\omega)) \]

\[ \Delta x \Delta p \geq \frac{\hbar}{2} \]

**Classical Mechanics**

**Quantum Mechanics**

**Path is deterministic**

**Path respects uncertainty relation**

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States of definite energy are stationary states

\[ i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(x,t) \]

\[ \Psi(x,t) = \chi(t) \psi(x) \]

Try set of solutions that allow the separation of \(x\) and \(t\).

\[ i\hbar \frac{\chi'(t)}{\chi(t)} = \frac{\hat{H}\psi(x)}{\psi(x)} = E. \]

This means that the **amplitude** of states of definite energy oscillate with time with frequency \(E/\hbar\).

\[ \Psi_E(x,t) = \psi_E(x) e^{-i \frac{E}{\hbar} t} \]

\[ |\Psi_E(x,t)|^2 = |\psi_E(x)|^2 \]

But observables relate to the probability, which is time independent \(\rightarrow\) this is why they are called **stationary states**.

• The energy eigenvalues of the time-independent Schrodinger equation are states of definite energy.
• Their probability density does not change with time \(\rightarrow\) they are called stationary states.
• This is analogous to the 1\textsuperscript{st} law of classical mechanics: quantum states of definite energy will continue to remain in those states unless perturbed by a potential.
Quantum mechanical current

\[ |\Psi(x, t)|^2 = \Psi^* \Psi \]

Probability density in space and time

\[ \frac{\partial |\Psi(x, t)|^2}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi \]

Change in probability density with time

\[ \frac{\partial |\Psi(x, t)|^2}{\partial t} = \Psi^* \left( \frac{\hat{p}^2}{2m} + V \right) \Psi + \Psi \left( \frac{\hat{p}^2}{2m} + V \right) \Psi^* \]

Use time-dependent Schrödinger equation

\[ \frac{\partial |\Psi(x, t)|^2}{\partial t} = \frac{1}{2mi\hbar} \left( \Psi^* \hat{p}^2 \Psi - \Psi \hat{p}^2 \Psi^* \right) \]

Since \( \hat{p} = -i\hbar \nabla_r \) \( \frac{\partial |\Psi(x, t)|^2}{\partial t} = -\nabla_r \cdot \left[ \frac{1}{2m} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*) \right] \)

Continuity equation

\[ \frac{\partial \rho}{\partial t} = -\nabla_r \cdot \mathbf{j} \]

\[ \mathbf{j} = \frac{1}{2m} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*) \]

Quantum mechanical probability current density

Satisfies the conservation of number of particles

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Electric current of quantum states

\[
J = \frac{q}{2m_e} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*)
\]

For most semiconductors we know the bandstructure, but not the Bloch functions. Go through the derivation to recast the current in terms of the bandstructure, or the group-velocity (see notes).

\[
J_d = \frac{q}{L^d} \sum_k v_g(k) f(k)
\]

\[
J_d = \frac{qg_s g_v}{L^d} \sum_k v_g(k) T(k) [f_L(k) - f_R(k)]
\]

\[
J_d = \frac{qg_s g_v}{(2\pi)^d} \int d^d k \times v_g(k) T(k) [f_L(k) - f_R(k)]
\]

\[v_g(k) = \nabla_k E(k)/\hbar\]

• Group velocity of electron in state \(|k>\)

VERY useful result: current in d-dimensions!

General expression for charge current density in d-dimensions
Quantum states are vectors in the Hilbert space

Any wavefunction \( \psi(x) = \sum \limits_n A_n \psi_n(x) \) is an allowed state.

Vector picture ⇒ \( |\psi> = \sum \limits_n A_n |n> \)

It is useful here to draw an analogy to the decomposition of a vector into specific coordinates. The ‘hybrid’ state function \( \psi(x) \) is pictured as a vector \(|\psi>\) in an abstract space. The definite momentum wavefunctions \( \psi_n(x) \) are pictured as the ‘coordinate’ vectors \(|n>\) in that space of vectors. This set of vectors is called the basis. Since there are an infinite set of integers \( n = 0, \pm 1, \pm 2, \ldots \), the vector space is infinite dimensional. It is called the Hilbert space. One may then consider the coefficients \( A_n \) as the length of the projections of the state on the basis states. The abstract picture allows great economy of expression by writing \( |\psi> = \sum \limits_n A_n |n> \). The orthogonality of the basis states

\[
|\psi> = \sum \limits_n A_n |n>
\]

\[
\langle m|n> = \delta_{mn}
\]

\[
A_n = \langle n|\psi>
\]

\[
|\psi> = \sum \limits_n \langle n|\psi> |n> = \sum \limits_n |n><n|\psi>
\]

\[
\sum \limits_n |n><n| = 1
\]
By projecting states, get various representations

We can think of the states as vectors.

The ‘inner product’ is a complex number generated by projection to the appropriate space.

This number is the wavefunction – it can be found in real space, momentum space, etc…
Outline

Part I: Review of fundamentals

1: Review of classical and quantum mechanics
2: Current flow in quantum mechanics
3: Quantum statistics, quest for equilibrium as the driver for transport

Part II: Single-particle transport

4: Ballistic transport: Quantized conductance, Ballistic MOSFETs
5: Transmission and tunneling, Tunneling FETs
6. Closed vs. open systems, the Non-Equilibrium Green’s Function approach to transport
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9: Fock-space way of thinking transport, second quantization, conductance anomalies
10: BCS theory of superconductivity, Josephson junctions
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13: Chern numbers, Edge/Topological states, Topological insulators and Majorana Fermions
Identity crisis: Indistinguishable particles

2 particles: total energy: \( E_1 + E_2 \Rightarrow \) time evolution \( e^{i(\frac{E_1+E_2}{\hbar}t)} \)

Since \( \frac{\partial}{\partial t} \psi = i\hbar \psi \), \( \psi \sim \psi_1 \cdot \psi_2 \)

\( e^{-\frac{E_1}{\hbar}t} \rightleftarrows e^{-\frac{E_2}{\hbar}t} \)

\( \psi(x_1, x_2) = \psi_a(x_1) \psi_b(x_2) \left\{ \begin{array}{ll} \text{OK for distinguishable!} & \text{but NOT OK for indistinguishable!!} \\ \end{array} \right. \)

\[ x_1 \leftrightarrow x_2 \text{ should NOT change the observables!} \]

This is OK for distinguishable particles such as a proton and an electron. But NOT OK for indistinguishable particles such as two electrons! For example, \(|\psi|^2\) should not change on swapping \( x_1 \leftrightarrow x_2 \).

How must we then write the wavefunction for two identical particles?
Resolution of identity crisis: Bosons & Fermions

This is necessary for indistinguishable particles.

\[ P(x_2, x_1) = P(x_1, x_2) \rightarrow |\psi(x_2, x_1)|^2 = |\psi(x_1, x_2)|^2. \]

\[ \psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) \]

\[ \psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) + \psi_a(x_2)\psi_b(x_1) \]

\[ \psi(x_2, x_1) = \psi(x_1, x_2) \]

\[ \psi(x_1, x_1) = \psi(x_1, x_1) \]

\[ \psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) - \psi_a(x_2)\psi_b(x_1) \]

\[ \psi(x_2, x_1) = -\psi(x_1, x_2), \]

\[ \psi(x_1, x_1) = -\psi(x_1, x_1) \rightarrow \psi(x_1, x_1) = 0. \]

The Pauli exclusion principle!

\[ f_{BE}(E) = \frac{1}{e^{\frac{E-\mu}{kT}}} \]

The Bose-Einstein distribution!

Particles are called **Bosons**.

Examples: Photons, Phonons

Bose

\[ f_{FD}(E) = \frac{1}{1 + e^{\frac{E-E_F}{kT}}} \]

The Fermi-Dirac distribution!

Particles are called **Fermions**.

Examples: Electrons, Protons

Fermi

• Note: Why not \[ \psi(x_2, x_1) = e^{i\phi}\psi(x_1, x_2) \] ? Majorana particles \( \rightarrow \) later…

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Quantum Statistical Mechanics in 1 slide

- Boltzmann equilibrium allows energy exchange without particles between reservoir and system.
- Gibb’s equilibrium allows energy and particle exchange between the reservoir and the system.
- The chemical potential is a measure of the number of particles.

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Fermi-Dirac and Bose-Einstein Distributions

- Both the Fermi-Dirac and Bose-Einstein distributions are for non-interacting particles.
- In the limit of high energies, they merge to the classical Boltzmann limit.

\[ f_{BE}(\mathcal{E}_i) = \frac{1}{e^{\beta(\mathcal{E}_i - \mu)} - 1} \]

\[ f_{FD}(\mathcal{E}_i) = \frac{1}{1 + e^{\beta(\mathcal{E}_i - \mu)}} \]

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**Fermi-Difference function and its integrals**

- The Fermi difference function will dominate our treatment of electron transport.
- The Fermi difference function looks like a box function with edges smeared with temperature.

\[
\int_0^\infty dE f_0(E - \mu) = \int_0^\infty \frac{dE}{1 + e^{\beta(E - \mu)}} = \frac{1}{\beta} \ln(1 + e^{\beta \mu}),
\]

\[
\int_0^\infty dE [f_0(E - \mu_1) - f_0(E - \mu_2)] = \frac{1}{\beta} \ln\left[\frac{1 + e^{\beta \mu_1}}{1 + e^{\beta \mu_2}}\right] = (\mu_1 - \mu_2) + \frac{1}{\beta} \ln\left[\frac{1 + e^{-\beta \mu_1}}{1 + e^{-\beta \mu_2}}\right].
\]

\[
\int_0^\infty dE [f_0(\mu_1) - f_0(\mu_2)] \approx (\mu_1 - \mu_2).
\]

\[
f(u) = 1/(1 + e^u) \quad \text{and} \quad f(v) = 1/(1 + e^v)
\]

\[
f(u) - f(v) = \left[ f(u) + f(v) - 2f(u)f(v) \right] \times \tanh\left(\frac{v - u}{2}\right)
\]

\[
\mu_1, \mu_2 \gg kT \quad \int_0^\infty dE [f_0(\mu_1) - f_0(\mu_2)] \approx (\mu_1 - \mu_2).
\]

**Figure 6.4:** Illustration of the temperature dependence of the Fermi-difference distribution. The difference is a window between \( \mu_2 - \mu_1 \) that becomes increasingly rectangular as the temperature drops.
Fermi-Dirac Integrals

The Fermi-Dirac Integrals (are moments) appear when we sum over states to calculate current.

The “order” of the integral is dependent on the dimensionality of the problem.

\[ F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty du \frac{u^j}{1 + e^{u-\eta}} \]

\[ F_j(\eta) \approx \begin{cases} e^\eta & \eta << -1 \\ \frac{\eta^{j+1}}{\Gamma(j+2)} & \eta >> 1 \end{cases} \]

**Figure 6.5**: Fermi-Dirac integrals and their non-degenerate (\(\eta << -1\)) and degenerate (\(\eta >> 1\)) approximations, illustrating Equation 6.20.
Equilibrium at contacts

• Electrons states in the metal contact reservoirs try bringing the “semiconductor” channel electron states in equilibrium with them by particle (or energy) transfer
• States in equilibrium share the same chemical potential, and their $f(k)$ is thus known
• Multiple contacts with different chemical potentials bring parts of channel states to equilibrium with themselves; the net current flows if there is an imbalance in current carrying states

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Equilibrium at multicarrier junctions

- Electrons states in the metal contact reservoirs try bringing the “semiconductor” channel electron states in equilibrium with them by particle (or energy) transfer.
- States in equilibrium share the same chemical potential, and their $f(k)$ is thus known.
- Multiple contacts with different chemical potentials bring parts of channel states to equilibrium with themselves; the net current flows if there is an imbalance in current carrying states.

**Figure 6.7:** Illustration of the concept of equilibrium for p-n junctions.
Equilibrium in Transistors

- Electrons states in the metal contact reservoirs try bringing the “semiconductor” channel electron states in equilibrium with them by particle (or energy) transfer
- States in equilibrium share the same chemical potential, and their $f(k)$ is thus known
- Multiple contacts with different chemical potentials bring parts of channel states to equilibrium with themselves; the net current flows if there is an imbalance in current carrying states

Figure 6.8: Illustration of the concept of equilibrium for a 3-terminal MOSFET
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Electron in a periodic potential (no analytic soln!)

We know the bandstructure, or $E(k)$ eigenvalues of the electron in the crystal.

Figure 13.2: Bandgap opening in the energy spectrum of a free electron upon perturbation by a periodic potential.
Effective Mass Approximation

- Effective Mass Approximation maps the complicated problem of Electrons in a complicated crystal + heterostructure potential ... to ... the simplest of all quantum mech problems: The particle in a box.

Motion of Electrons and Holes in Perturbed Periodic Fields

J. M. Luttinger* and W. Kohn
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received October 13, 1954)

A new method of developing an “effective-mass” equation for electrons moving in a perturbed periodic structure is discussed. This method is particularly adapted to such problems as arise in connection with impurity states and cyclotron resonance in semiconductors such as Si and Ge. The resulting theory generalizes the usual effective-mass treatment to the case where a band minimum is not at the center of the Brillouin zone, and also to the case where the band is degenerate. The latter is particularly striking, the usual Wannier equation being replaced by a set of coupled differential equations.

- Developed by Luttinger & Kohn and refined since then...
- Real power of the EMA is exercised in understanding the electronic properties of Quantum Heterostructures.
Effective Mass Approximation

\[ E_n(k) \approx E_c(r) + \frac{\hbar^2 k^2}{2m^*} \rightarrow E_n(-i\nabla) \approx E_c(r) - \frac{\hbar^2}{2m^*} \nabla^2 \]

\[ \left[ -\frac{\hbar^2}{2m^*} \nabla^2 + V_{imp}(r) \right] C(r) = \left[ E - E_c(r) \right] C(r) \]

Central Result of Effective Mass Approximation

“Particle-in-a-box” problem with:
- Real mass -> Effective mass,
- Real wavefunction -> Envelope function
- Crystal potential -> Band-edge potential + Impurity potentials, etc

Example: Shallow donor states

\[ \left[ -\frac{\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{4\pi \varepsilon r} \right] C(r) = (E - E_c) C(r) \]

\[ E - E_c = E_\infty \frac{m^*}{\varepsilon_r^2} \]

\[ a_B^* = a_B \frac{\varepsilon_r}{m^*} \]

\[ C(r) \sim e^{-r/\tau_0} \]
Density of States

\[ g(\varepsilon) = g_s \cdot \sum_{\mathbf{k}} \delta[\varepsilon - \varepsilon(\mathbf{k})] \]

Valid for electrons, photons, phonons...

Important result: \[ \sum_{\mathbf{k}} (...) \rightarrow \int \frac{d^d\mathbf{k}}{(2\pi)^d} (...) \]

If we know the energy dispersion \( \varepsilon(\mathbf{k}) \), we can find the DOS using this prescription.

Free Electron: \( \varepsilon(\mathbf{k}) = \frac{\hbar^2|\mathbf{k}|^2}{2m_0} \)
Free electron in 3D: \( g(\varepsilon) = g_s \cdot \frac{1}{(2\pi)^2} \left( \frac{2m_0}{\hbar^2} \right)^{3/2} \sqrt{\varepsilon} \)
Effective Mass Approximation

Application: Bulk Semiconductors

• 3D (Bulk)

\[
\begin{align*}
[-\frac{\hbar^2}{2m^*} \nabla^2 + V_{np}(r)] C(r) &= [E - E_{c}(r)] C(r) \\
C(r) &= \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}} \\
E(k) &= E_{c0}(r) + \frac{\hbar^2 k^2}{2m^*} = E_{c0}(r) + \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_{xx}^*} + \frac{k_y^2}{m_{yy}^*} + \frac{k_z^2}{m_{zz}^*} \right)
\end{align*}
\]

\[
g_{3D}(E) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_{c0}}
\]

\[
n = \int_0^\infty dE f_{FD}(E) g_{3D}(E) = N_C^{3D} F_{1/2} \left( \frac{E_C - E_F}{k_B T} \right) \approx N_C^{3D} e^{-\frac{E_C - E_F}{k_B T}}
\]
Effective Mass Approximation

\( \cdot 2D \) (Quantum Wells)

\[ V(x, y, z) = 0, \quad z < 0 \]
\[ V(x, y, z) = 0, \quad z > W \]
\[ V(x, y, z) = -\Delta E_c, \quad 0 \leq z \leq W. \]

\[ k_{n_z} = \frac{\pi}{W} n_z \]

\[ C_{n_z}(x, y, z) = \phi(x, y) \chi_{n_z}(z) = \left[ \frac{1}{\sqrt{A}} e^{i(k_x x + k_y y)} \right] \cdot \left[ \chi_{n_z}(z) \right] \]

\[ E(k) = E_{c0} + \frac{\hbar^2}{2m^*_{xx}} \left( \frac{k_x^2}{m^*_{xx}} + \frac{k_y^2}{m^*_{yy}} \right) + \frac{\hbar^2}{2m^*_{zz}} \left( \frac{\pi n_z}{W} \right)^2 \]

\[ g_{2D}(E) = \frac{m^*}{\pi \hbar^2} \sum_{n_z} \theta(E - E_{n_z}) \]

\[ n_{2D} = \int_0^\infty dE f_{FD}(E) g_{2D}(E) = \frac{m^* k_B T}{\pi \hbar^2} \ln \left( 1 + e^{\frac{E_F - E_1}{k_B T}} \right) \]

\[ n_{2D} = \sum_i n_j = N_c^{2D} \sum_j \ln \left( 1 + e^{\frac{E_j - E_1}{k_B T}} \right) \]
Effective Mass Approximation

- **1D (Quantum Wires)**

\[ k_{n_x} = \frac{\pi}{L_x} n_x, \]
\[ k_{n_y} = \frac{\pi}{L_y} n_y, \]
\[ C(x, y, z) = \chi_{n_x}(x) \cdot \chi_{n_y}(y) \cdot \left( \frac{1}{\sqrt{L_z}} e^{ik_x x} \right) \]
\[ E(n_x, n_y, k_z) = E(n_x, n_y) + \frac{\hbar^2 k_z^2}{2m_{zz}^*} \]

Figure 3: Bandstructure, and DOS of realistic quantum wires.

\[ C_{n_x, n_y}(x, y, z) = \left[ \sqrt{\frac{2}{L_x}} \sin\left( \frac{\pi n_x}{L_x} x \right) \right] \cdot \left[ \sqrt{\frac{2}{L_y}} \sin\left( \frac{\pi n_y}{L_y} y \right) \right] \cdot \left[ \frac{1}{\sqrt{L_z}} e^{ik_x x} \right] \]

\[ E(n_x, n_y, k_z) = \left[ \frac{\hbar^2}{2m_{xx}} \left( \frac{\pi n_x}{L_x} \right)^2 \right] + \left[ \frac{\hbar^2}{2m_{yy}} \left( \frac{\pi n_y}{L_y} \right)^2 \right] + \frac{\hbar^2 k_z^2}{2m_{zz}^*} \]

\[ g_{1D}(E) = \frac{1}{\pi} \sqrt{\frac{2m^*}{\hbar^2}} \frac{1}{\sqrt{E - E_1}} \]

\[ g_{QWire}(E) = \frac{1}{\pi} \sqrt{\frac{2m^*}{\hbar^2}} \sum_{n_x, n_y} \frac{1}{\sqrt{E - E(n_x, n_y)}} \]
Effective Mass Approximation

- **0D (Quantum Dots)**

\[
C(x, y, z) = \left[ \sqrt{\frac{2}{L_x}} \sin\left(\frac{\pi n_x}{L_x}\right) \right] \cdot \left[ \sqrt{\frac{2}{L_y}} \sin\left(\frac{\pi n_y}{L_y}\right) \right] \cdot \left[ \sqrt{\frac{2}{L_z}} \sin\left(\frac{\pi n_z}{L_z}\right) \right]
\]

\[
E(n_x, n_y, n_z) = \frac{\hbar^2}{2m_{xx}} \left(\frac{\pi n_x}{L_x}\right)^2 + \frac{\hbar^2}{2m_{yy}} \left(\frac{\pi n_y}{L_y}\right)^2 + \frac{\hbar^2}{2m_{zz}} \left(\frac{\pi n_z}{L_z}\right)^2
\]

\[
g_{QDot} = \sum_{n_x, n_y, n_z} \delta(E - E_{n_x, n_y, n_z})
\]

Figure 4: Energy levels and DOS of quantum dots.
Effective Mass Theory works even at sharp heterojunctions, and it works amazingly well! Quantum cascade lasers are designed using this theory.

Proof presented in:
Burt, APL 65 717 (1994)
Example: Exciton in an InN Nanowire

$$\left| C(r) \right|^2$$

envelope function

$$\left| \Psi(r) \right|^2 = \left| C(r) \right|^2 \times \left| u(r) \right|^2$$

exciton

Bloch function

Nanowire

Nano Letters (2014)

E. Kioupakis et al. (Michigan)

Debdeep Jena (djena@cornell.edu), Cornell University
Perfect Crystal: ‘Bloch’ single electron transport

**Perfect Crystalline Materials**

- Bloch oscillations

\[ \mathbf{F} = (-e) \cdot [\mathbf{E} + \mathbf{v} \times \mathbf{B}] = \hbar \frac{dk}{dt} \]

\[ \mathbf{v} = \frac{1}{\hbar} \frac{\partial E(k)}{\partial k} = \frac{1}{\hbar} \nabla_k E(k) \]

\[ \mathbf{a} = \frac{\mathbf{F}}{m^*} \]

\[ \mathbf{v} = \frac{d\mathbf{r}}{dt} \]

A static periodic potential causes no scattering.

Umklapp process

‘One’ electron: Bloch oscillations

Can easily transform to real space.
Most general expression for ‘Current Density’ in ‘d’ dimensions:

\[ \mathbf{J}_d = q \times \frac{g_s g_v}{L^d} \sum_k \mathbf{v}_g(k) f(k), \]

where

- \( g_s = \) spin degeneracy
- \( g_v = \) valley degeneracy

\( \mathbf{v}_g = \frac{1}{\hbar} \nabla \mathcal{E}(\mathbf{k}) \) is the group velocity

\( f(k) \) is the Fermi-Dirac function

Example: 1D current flow at \( T = 0 \text{ K} \):

\[ J_1 = I = I_{\rightarrow} - I_{\leftarrow} \]
\[ I_{\rightarrow} = \frac{2q}{\hbar} E_{F1} \]
\[ I_{\leftarrow} = \frac{2q}{\hbar} E_{F2} \]

\[ \rightarrow I = I_{\rightarrow} - I_{\leftarrow} = \frac{2q^2}{\hbar} V_D \]
“Ballistic” Transport & Quantized Conductance

Experiments:

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).

FIG. 1. (a) Schematic layer structure of the heterostructure. (b) Improvement of plateau quantization with the application of a small magnetic field. Linear conductance $G(V_g)$ is plotted at magnetic field $B=0.1$ T, 0.2 T, 0.5 T, and 1 T. Traces are shifted vertically for clarity. Inset: micrograph of the QPC. The gap between the two split gates is 80 nm at its narrowest point. All experimental data shown in this letter were measured at 300 mK.

Contact resistances are at the quantum limit!

MBE-Regrown Ohmics in InAlN HEMTs With a Regrowth Interface Resistance of 0.05 Ω · mm

Jia Guo, Student Member, IEEE, Guowang Li, Student Member, IEEE, Faiza Faria, Yu Cao, Ronghua Wang, Jai Verma, Xiang Guo, Shipping Guo, Member, IEEE, Edward Beem, Andrew Ketterson, Michael Schuette, Member, IEEE, Paul Saunier, Senior Member, IEEE, Mark Wister, Member, IEEE, Debdeep Jena, Member, IEEE, and Huili Xing, Member, IEEE

Contact resistances are at the quantum limit!

- MBE grown ohmic contacts are a key enabler of high RF performance
- Various groups (e.g. HRL) have adopted AlN/GaN MBE HEMT technology

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From Ballistic conductance to Ohm’s Law

\[ R_0 \sim \frac{h}{2q^2} \]

\[ G_0 \sim \frac{2q^2}{h} \]

\[ R = \rho \frac{L}{A} \]

\[ G = \sigma \frac{A}{L} \]

For \( L \gg \lambda_{mfp} \) and 3D: \( M \sim k_F^2 A \)

\[ \rightarrow R \sim \frac{h}{2q^2} \cdot \frac{1}{k_F^2 A} \cdot \frac{L}{\lambda_{mfp}} \quad \text{(Ohm’s Law)} \]

For \( L \ll \lambda_{mfp} \) and 3D: \( M \sim k_F^2 A \)

\[ \rightarrow R \sim \frac{h}{2q^2} \cdot \frac{1}{k_F^2 A} \quad \text{(Sharvin resistance)} \]
Ballistic Field-Effect Transistor

Debdeep Jena (djena@cornell.edu), Cornell University
• The physics of a Ballistic FET can be understood by inspecting the carrier distribution in k-space at the source-injection Point.

Debdeep Jena (djena@cornell.edu), Cornell University
Figure 1: Field effect transistor, energy band diagram, and k-space occupation of states.
Ballistic Field-Effect Transistor

Figure 2: Field effect transistor, energy band diagram, and \( k \)-space occupation of states.
Ballistic Field-Effect Transistor

\[
\frac{q^2 n_s}{C_b} + kT \ln \left( e^{\frac{q n_s}{e C_q V_{th}}} - 1 \right) = q(V_{gs} - V_T) \implies e^{\frac{q n_s}{e C_q V_{th}}} (e^{\frac{q n_s}{e C_q V_{th}}} - 1) = e^{\frac{V_{gs} - V_T}{V_{th}}}
\]

**FIGURE 10.2:** Illustrating the dependence of the 2DEG sheet density at the injection point on the gate voltage.

2D electron gas density at the injection point of a FET as a function of the gate voltage
Ballistic Field-Effect Transistor

- Ballistic FETs are much simpler to understand than long-channel devices based on drift/diffusion.

- 2DEG electron density dependence on $V_{ds}$ & $V_g$

$$n_{inj} = n_R + n_L = \frac{g_s g_v m^* kT}{4\pi \hbar^2} \left[ \ln(1 + e^{E_{fs}}) + \ln(1 + e^{E_{fd}}) \right]$$

Thus, $q n_{inj} = C_{gs} (V_{gs} - V_t)$, and $E_{fs} - E_{fd} = q V_{ds}$. Solve these two equations and show that the source quasi-Fermi-level is related to the gate and drain biases through the relation

$$v_s = \frac{E_{fs}}{kT} = \ln\left[ \sqrt{(1 + e^{v_d})^2 + 4e^{v_d}(e^\rho - 1) - (1 + e^{v_d})} \right] - \ln[2], \quad (4)$$

where $v_d = V_{ds}/kT$ and $\rho = 4\pi \hbar^2 C_{gs} (V_{gs} - V_t)/q g_s g_v m^* kT$.

$$\frac{I_d}{W} = q \frac{g_s g_v}{(2\pi)^2} \frac{\hbar}{m^*} \left( \frac{2m^* kT}{\hbar^2} \right)^{\frac{3}{2}} \left[ F_{1/2}(v_s) - F_{1/2}(v_s - v_d) \right], \quad (5)$$

where $F_j(x) = 1/\Gamma(j + 1) \int_0^\infty y^j (1 + \exp[y - x])^{-1} dy$ is the Fermi-Dirac integral of order $j$. 

Debdeep Jena (djena@cornell.edu), Cornell University
Ballistic Field-Effect Transistor

\[ n_q = q^2 D_0 V_{th} = C_q V_{th} \]

\[ D_0 = g_s \cdot g_v \frac{m_c^*}{2\pi \hbar^2} \]

\[ \eta_s = \ln[\sqrt{(1 + e^{v_d})^2 + 4e^{v_d}(e^{2n_s(V_{gs}/n_q - 1)} - (1 + e^{v_d}))} - 1] - \ln 2 \]

\[ J_0 = \frac{qg_sg_v \sqrt{2m_c^*}}{2\pi^2 \hbar^2} (kT)^{3/2} \]

\[ I_d / W = \frac{1}{2} \left[ F_{1/2}(\eta_s) - F_{1/2}(\eta_d) \right] \]

Debdeep Jena (djena@cornell.edu), Cornell University
Ballistic Field-Effect Transistor

\[ I_d = e \left( e^{V_{gs} - V_T} - 1 \right) = e^{V_{th}} \]

\[ n_b = C_b V_{th} \]

\[ C_b = \varepsilon_b / t_b \]

\[ n_q = q^2 D_0 V_{th} = C_q V_{th} \]

\[ D_0 = g_s \cdot g_v \frac{m^*}{2\pi\hbar^2} \]

\[ \eta_s = \ln[\sqrt{(1 + e^{V_d})^2 + 4e^{V_d} (e^{2n_s(V_{gs})/n_q} - 1) - (1 + e^{V_d})}] - \ln 2 \]

\[ J_0 = \frac{qg_s g_v \sqrt{2m^*}}{2\pi^2 h^2} (kT)^{3/2} \]

\[ I_d / W = \begin{cases} J_0 [F_{1/2} (\eta_s) - F_{1/2} (\eta_d)] \end{cases} \]

\[ F_j(\eta) = \frac{1}{\Gamma(j + 1)} \int_0^\infty du \frac{u^j}{1 + e^{u-\eta}} \]

\[ F_j(\eta) \approx \begin{cases} e^{-\eta} & \eta < 1 \\ \eta^{j+1} & \eta >> 1 \end{cases} \]

\[ \frac{I_d}{W} \sim J_0 e^{\frac{V_{gs} - V_T}{V_{th}}} \]

\[ \frac{I_d}{W} \sim J_0 \left( \frac{V_{gs} - V_T}{V_{th}} \right)^{3/2} \]

Subthreshold (off)

On-state
Silicon Ballistic Field-Effect Transistor

Figure 10.4: Ballistic Silicon FET. The device dimensions are $t_b = 1$ nm, $\epsilon_b = 10\epsilon_0$, and for Silicon, $m^* = 0.2m_0$ and $g_v = 2.5$ are used.

- Note the on-off ratio, and the sharper switching at low temperatures. The subthreshold slope is $\sim(kT/q)\ln(10)$.
- This calculation neglects the contact resistance incurred in injecting carriers from 3D source to 2D channel.

Debdeep Jena (djena@cornell.edu), Cornell University
Silicon Ballistic Field-Effect Transistor

- injection velocity (ensemble averaged)

FIG. 5. Calculated examples of I-V characteristics of an nMOSFET on (100) plane. $C_{\text{eff}}$ corresponds to effective 5 nm oxide thickness: (a) channel current per unit width vs drain voltage, parameter is the gate voltage; (b) channel current per unit width versus gate voltage, parameter is the drain voltage.

FIG. 8. Saturation current per unit width and the injection velocity of an nMOSFET on (100) plane as functions of inversion carrier density. The current value gives the maximum limit of the MOSFET current.

\[ v_{\text{inj}} = \frac{I_{\text{sat}}}{WC_{\text{eff}}(V_G - V_t)}, \]  \hspace{1cm} (31)

\[ v_{\text{inj}} = \frac{8h \sqrt{|Q|}}{3m_t \sqrt{q} \pi M_v} = \frac{8h \sqrt{C_{\text{eff}}(V_G - V_t)}}{3m_t \sqrt{q} \pi M_v} \]  \hspace{1cm} (32)

When the carriers towards the drain are degenerate. This value is consistent with the fact that the propagating state towards the drain is occupied at $x_{\text{max}}$ up to those with the velocity $v_f$. 
Space-charge transport of electrons

The saturated current, Eq. (24), is proportional to $(V_G - V_t)^{3/2}$ since the carrier mean velocity is proportional to $\sqrt{Q}$, as is the Fermi velocity. The fact that carriers are degenerate Fermi particles plays an important role here. This is in contrast with the classical MOSFET where the saturated current is proportional to $(V_G - V_t)^2$ or $(V_G - V_d)$.

The ballisitic current in the bulk material reminds us of the space-charge limited current expressed by the $3/2$ power law of Langmuir’s equation. The geometry of the MOSFET is different from those that are assumed in these bulk type current structures, but a similar simple discussion is attempted so that we may be able to gain some insight into the resultant potential variation along the channel. Suppose that the carrier transport is ballistic and the channel length is not as short. The channel potential variation along the $x$ axis measured from the value at the source edge is denoted by $\Delta \phi(x) \ [\Delta \phi(0) = 0]$. The carrier mean velocity at $x, v(x)$, is related to $\Delta \phi(x)$ as

$$\frac{1}{2}mv(0)^2 = \frac{1}{2}mv(x)^2 + \Delta \phi(x), \quad (34)$$

where $m$ is the carrier effective mass. The current continuity condition requires that

$$I = qWn(x)v(x). \quad (35)$$

1) Ballistic Limit: $J_{ballistic}^{sc} \propto V^{3/2}$

2) Mott-Gurney, diffusive limit: $J_{diff}^{sc} \propto V^2$

3) Saturated diffusive limit: $J_{sat}^{sc} \propto V$
A 2D Crystal Channel Ballistic FET

- Note the on-off ratio, and the sharper switching at low temperatures. The subthreshold slope is \( \sim (kT/q) \ln(10) \).
- This calculation neglects the contact resistance incurred in injecting carriers from 3D source to 2D channel.

\[
I_d/V, \text{mA/micron} = \begin{cases} 
10^{-7} & \text{off} \\
10^{-3} & \text{on}
\end{cases}
\]

\[
\frac{V_{gs}-V_T}{V_{th}} \ll -1 \\
\frac{V_{gs}-V_T}{V_{th}} \gg +1
\]

\[
n_s \approx \left( \frac{C_q V_{th}}{q} \right) \cdot e^{-\frac{V_{gs}-V_T}{V_{th}}}
\]

\[
n_s \approx \frac{1}{q} \frac{C_b C_q}{C_b + C_q} (V_{gs} - V_T)
\]

Debdeep Jena (djena@cornell.edu), Cornell University
How can one go below the 60 mV/decade limit?
How good can GaN TFETs be?

- Tunnel-FETs have the potential to beat the 60 mV/decade limit in switching

Debdeep Jena (djena@cornell.edu), Cornell University
Outline

- **Part I: Review of fundamentals**
  1. Review of classical and quantum mechanics
  2. Current flow in quantum mechanics
  3. Quantum statistics, quest for equilibrium as the driver for transport

- **Part II: Single-particle transport**
  4. Ballistic transport: Quantized conductance, Ballistic MOSFETs
  5. Transmission and tunneling, Tunneling FETs
  6. Closed vs. open systems, the Non-Equilibrium Green’s Function approach to transport
  7. Diffusive transport: Boltzmann transport equation, scattering, electron-phonon interactions
  8. High-field effects, Gunn diodes and oscillators for high-frequency power

- **Part III: Many-particle correlated transport**
  9. Fock-space way of thinking transport, second quantization, conductance anomalies
  10. BCS theory of superconductivity, Josephson junctions
  11. Landau/Ginzburg theories of phase transitions due to broken symmetry

- **Part III: Geometrical and topological quantum mechanics, unification with relativity**
  12. Spin, transport in a magnetic field, Quantum Hall effect, Berry phase in quantum mech
  13. Chern numbers, Edge/Topological states, Topological insulators and Majorana Fermions
Why can electrons tunnel through barriers?

- Photons

Total internal reflection
Why can electrons tunnel through barriers?

photons

Total internal reflection

Debdeep Jena (djena@cornell.edu), Cornell University
Why can electrons tunnel through barriers?

- photons
- Total internal reflection
- "tunneling of photons"
Why can electrons tunnel through barriers?

**Total internal reflection**

**De Broglie**

\[ \lambda = \frac{h}{mv} \]

Reflection of electron wave

“tunneling of photons”
Why can electrons tunnel through barriers?

Total internal reflection

De Broglie

$\lambda = \frac{h}{mv}$

Reflection of electron wave

“tunneling of electrons”

“tunneling of photons”
Tunneling Transport in Semiconductors

Goals:

To learn
• Historical development of ideas of quantum mechanical tunneling
• Tunneling concepts in solids: a single-particle picture
• Existing models for calculating tunneling currents
• Intraband tunneling and resonant tunneling diodes
• Interband (Zener) tunneling in pure semiconductors
• Zener tunneling mediated by phonons, defects, or other perturbations
• The Tunnel-Field Effect Transistor (TFET)
One might think ... that imaginary numbers are just a mathematical game having nothing to do with the real world. From the viewpoint of positivist philosophy, however, one cannot determine what is real. All one can do is find which mathematical models describe the universe we live in. It turns out that a mathematical model involving imaginary time predicts not only effects we have already observed but also effects we have not been able to measure yet nevertheless believe in for other reasons. So what is real and what is imaginary? Is the distinction just in our minds? - Stephen Hawking
3) Total internal reflection & Evanescent waves (7 Points):

We have discussed the case of total internal reflection when an EMag wave is incident from a material of high dielectric constant to a material of lower dielectric constant. Though the energy is reflected back, a certain part of the EMag wave leaks out into the low dielectric constant medium and moves parallel to the interface; this part is called the ‘evanescent’ wave.

Consider the case of an EMag wave incident from a non-magnetic region with $\epsilon_1 = 4$ to say air ($\epsilon_2 = 1$) as indicated in Figure 2.

(a) Find the critical angle for total internal reflection $\theta_c$.

(b) Now assume that the wave is incident at an angle $15^\circ$ larger than the critical angle: $\theta_1 = \theta_c + 15^\circ$, and its wavevector is $\beta_1$. Write down the components of the transmitted wavevector $\beta_2$ in the $z$- and $x$-directions. In particular, show using Snell’s law that the $x$-component of $\beta_2$ becomes imaginary.

\[
\begin{align*}
\nabla^2 E - \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} &= 0, & \text{Wave Equations} \\
\nabla^2 B - \frac{1}{c^2} \frac{\partial^2 B}{\partial t^2} &= 0.
\end{align*}
\]

\[
\psi(x,t) =\frac{e^{i(k \cdot r - \omega t)}}{\beta}
\]

\[
\Psi(x,t) \propto e^{i(k \cdot r - \omega t)}
\]

Maxwell’s equations for photons (waves) have solutions with imaginary wavevectors $\rightarrow$ And the effects are REAL: Skin depth, Evanescent waves $\rightarrow$ If electrons have wave-like nature, they should exhibit similar phenomena

(c) Now show that in region 2, there is an evanescent wave whose electric field decays in the $z-$direction as $e^{-\alpha z}$ where $\alpha = |\beta_2| \sqrt{\frac{\epsilon_2}{\epsilon_1}} \sin^2 \theta_1 - 1$, but propagates along the $x-$direction. What does this mean for energy carried by the evanescent mode in the $z-$ and $x-$directions?

(d) Find the characteristic length of the decay of the intensity of the evanescent wave, where the intensity drops by a factor $1/e$. Recall that intensity goes as square of the electric field amplitude.

(Note for after the exam: This principle has been used for making a hybrid silicon evanescent laser. Silicon is notoriously difficult to make into a laser, so researchers have done the next big thing - used a III-V semiconductor laser and bonded it to Silicon so that the evanescent portion of the laser light is in Silicon, and is then waveguided using Silicon to different parts of the chip or from one core to another. Another interesting analogy is the following: the evanescent nature of the photons of an EMag wave is similar to the phenomena of quantum mechanical tunneling of electrons across forbidden barriers.)
## History of Tunneling

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### Alpha decay

From Wikipedia, the free encyclopedia

**Alpha decay**, or α-decay, is a type of radioactive decay in which an atomic nucleus emits an alpha particle and thereby transforms (or ‘decays’) into an atom with a mass number 4 less and atomic number 2 less. For example, uranium-238 decaying through α-particle emission to form thorium-234 can be expressed as:

\[
^{238}_{92}U \rightarrow ^{234}_{90}Th + \alpha
\]

### History

Alpha particles were first described in the investigations of radioactivity by Ernest Rutherford in 1899, and by 1907 they were identified as He²⁺ ions. For more details of this early work, see Alpha particle#History of discovery and use.

By 1928, George Gamow had solved the theory of the alpha decay via tunneling. The alpha particle is trapped in a potential well by the nucleus. Classically, it is forbidden to escape, but according to the (then) newly-discovered principles of quantum mechanics, it has a tiny (but non-zero) probability of “tunneling” through the barrier and appearing on the other side to escape the nucleus. Gamow solved a model potential for the nucleus and derived, from first principles, a relationship between the half-life of the decay, and the energy of the emission, which had been previously discovered empirically, and was known as the Geiger–Nuttall law.¹²
History of Tunneling

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Electron Emission in Intense Electric Fields.

By R. H. Fowler, F.R.S., and Dr. L. Nordheim.

(Received March 31, 1925.)

§ 1. Introduction.—The main features of the phenomenon of the extraction of electrons from cold metals by intense electric fields are well known, and an approximate theory of the effect was first developed by Schottky. More recently the experimental data have been much improved, notably by Millikan and Eyring, and Millikan and Lauritsen. The theory has been considered afresh by O. W. Richardson and by Houston: working with Sommerfeld.

Field-ionization of metals

Fig. 2.
# History of Tunneling

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**Non-Adiabatic Crossing of Energy Levels.**

By CLARENCE ZENER, National Research Fellow of U.S.A.

(Communicated by R. H. Fowler, F.R.S.—Received July 19, 1932.)

1. Introduction.

The crossing of energy levels has been a matter of considerable discussion. The essential features may be illustrated in the crossing of a polar and homopolar state of a molecule.

---

**A Theory of the Electrical Breakdown of Solid Dielectrics**

Clarence Zener

*Proc. R. Soc. Lond. A* 1934
doi: 10.1098/rspa.1934.011

---

**Fig. 1.—“Potential barrier” diagram.** The shaded regions represent zones of forbidden energy in the presence of an electric field.
**History of Tunneling**

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**New Phenomenon in Narrow Germanium p-n Junctions**

**LEO ESAMI**

_Tokyo Tsushin Kogyo, Limited, Shinagawa, Tok. Yamato_

(Received October 11, 1957)

**Interband tunneling in semiconductor diodes**

\[
I = I_{e \rightarrow v} - I_{v \rightarrow e} = A \int_{E_c}^{E_F} \{ f_{c}(E) - f_{v}(E) \} Z \rho_{c}(E) \rho_{v}(E) dE.
\]
### History of Tunneling

#### Table 1: Landmarks in the Science of Tunnelling

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**Giaever**

**Bardeen**

**Tunneling of Cooper pairs in S-I-S junctions: Experimental verification of the BCS theory and method to measure the superconducting gap**
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### Applications:
- SEMs
- TEMs
- STMs
- Tunnel diodes
- Ohmic contacts
- RTDs
- Quantum Cascade Lasers
- TFETs...

---

**The Nobel Prize in Physics 1973**

Leo Esaki, Ivar Giaever, Brian D. Josephson

- Nobel Prize Award Ceremony
- Leo Esaki
- Ivar Giaever
- Brian D. Josephson

**The Nobel Prize in Physics 1986**

Ernst Ruska, Gerd Binnig, Heinrich Rohrer

- Nobel Prize Award Ceremony
- Ernst Ruska
- Gerd Binnig
- Heinrich Rohrer

Ernst Ruska, Gerd Binnig, Heinrich Rohrer

The Nobel Prize in Physics 1986 was divided, one half jointly to Ernst Ruska “for his fundamental work in electron optics, and for the design of the first electron microscope”, the other half jointly to Gerd Binnig and Heinrich Rohrer “for their design of the scanning tunneling microscope”.

---

Debdeep Jena (djena@cornell.edu), Cornell University 95/xx
Tunneling Transmission: Exact

\[ T(E) = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)} \sin^2(k_b a)} \]
\[ k_b = \sqrt{\frac{2m}{\hbar^2}}(E - V_0) \]

For \( E < V_0 \), \( k_b = i \kappa_b \)
\[ \sin(iy) = i \sinh(y) \]

\[ T(E) = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)} \sinh^2(\kappa_b a)} \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa_b a} \]

For \( \kappa a >> 1 \)

• In the limit of thick barriers, we recover a WKB-type approximate result from the exact form

Debdeep Jena (djena@cornell.edu), Cornell University
The WKB result is the “classical” limit of the Feynman path integral; it neglects interference.
Tunneling Currents: Jump Start

A back-of-the-envelope evaluation of interband tunneling current in semiconductors

\[ T_{WKB} \sim e^{-2S} \]

\[ S = \int_{x_1}^{x_2} \sqrt{\frac{2m^*}{\hbar^2} (E_g - eFx)} \, dx \]

\[ x_1 = 0, x_2 = \frac{E_g}{eF} \]

\[ \implies T_{WKB} \sim \exp\left[-\frac{2\frac{5}{3} \sqrt{m^*} \, E_g^\frac{3}{2}}{3eFh}\right] = \exp\left[-\frac{F_0}{F}\right] \]

\[ \hbar \frac{dk}{dt} = eF \implies k(t) = k(0) + \frac{eF}{\hbar} t \]

\[ \implies \text{Bloch Osc. period: } T = \frac{\hbar G}{eF} \]

Rate of incidence on band-edge:

\[ \gamma_{inc} = \frac{1}{T} = \frac{eF}{\hbar G} = \frac{a_0 eF}{\hbar}, \]

where \( G = 2\pi/a_0 \) is the reciprocal lattice vector.

Frequency of electron escape:

\[ f_{esc} \sim \gamma_{inc} T_{WKB} = \frac{a_0 eF}{\hbar} \times \exp\left[-\frac{2\frac{5}{3} \sqrt{m^*} \, E_g^\frac{3}{2}}{3eFh}\right] \]

Tunneling current density:

\[ J_T \sim eN_s f_{esc} = eN_v x_{win} f_{esc} = eN_v (eV/F) f_{esc} \]

\[ \implies J_T \sim \frac{e^2}{h} \cdot [a_0 N_v \exp\left[-\frac{2\frac{5}{3} \sqrt{m^*} \, E_g^\frac{3}{2}}{3eFh}\right]] \cdot V \]
Tunneling Current

Kane’s method:

\[ \varepsilon - U = -\frac{(\varepsilon_0/2)^2 - \varepsilon_c^2}{\varepsilon_0} \]

\[ \varepsilon_{\parallel} - U = -\left[ \frac{(\varepsilon_0/2)^2 - \varepsilon_c^2}{\varepsilon_0} + \varepsilon_\perp \right] \]

\[ f = \int_{a'}^{b'} \left| \frac{2m}{\hbar^2} \left[ \frac{(\varepsilon_0/2)^2 - \varepsilon_c^2}{\varepsilon_0} + \varepsilon_\perp \right] \right|^{1/4} dx \]

\[ \varepsilon_c = qEx \]

\[ P = e^{-2f} = P_0 \exp \frac{-\varepsilon_1}{\varepsilon} \]

\[ P_0 = \exp \left( -\frac{\pi m^* \varepsilon_0}{2 \sqrt{2} q Eh} \right) = \exp \frac{-\varepsilon_0}{4\varepsilon} \]

\[ \varepsilon = \frac{\sqrt{2} q Eh}{2\pi m^* \varepsilon_0} \]

Moll (Physics of Semiconductors)

Tunneling current with lateral momentum conservation

Fig. 13-4 If the band gap is \( \varepsilon_0 \) and the field is \( E \), then \( b - a = \varepsilon_0 / qE \). If \( \varepsilon_1 > 0 \), the tunneling probability is reduced since the forbidden region extends from \( a' \) to \( b' \).
Tunneling probability in 3D semiconductors:

\[ T(k_\parallel) = T_0 \exp\left[ -c_0 \sqrt{\frac{m^*}{\hbar eF}} E_g^{3/2} \right] \exp\left[ -\frac{E_\parallel}{\bar{E}_k} \right] \]

where \( T_0 \) and \( c_0 \) are of the order of 1.

\[ E_\parallel = \frac{\hbar^2 (k_\parallel - k_0, \parallel)^2}{2m^*} \]

Electrons in states with \( k_\parallel \neq 0 \) see an effectively larger gap, and their tunneling probability is hence exponentially damped with energy. Expressions for \( \bar{E}_k \) depend on the chosen bandstructure model.

For a 2-band \( k \cdot p \) model:

\[ \left( \begin{array}{cc} E_g + \frac{\hbar^2 k^2}{2m_0} & \frac{\hbar k \cdot p}{m_0} \\ \frac{\hbar k \cdot p}{m_0} & \frac{\hbar^2 k^2}{2m_0} \end{array} \right) \]

\[ T_0 = \left( \frac{\pi}{3} \right)^2, \quad c_0 = \frac{\pi}{2^{3/2}}, \quad m^* = \frac{m_0^2 E_g}{2p_{cv}^2} \]

\[ \bar{E}_k = \frac{2^{1/2} \hbar eF}{2\pi \sqrt{m^* \sqrt{E_g}}} \]

As before, the momentum matrix element of most semiconductors satisfy the relation \( 2p_{cv}^2 / m_0 \approx 20 \text{ eV} \).
Tunneling Current: with lateral ‘k’ conservation

Procedure for calculating tunneling current:

Energy + lateral momentum conservation:
\[ E_v^p - \frac{\hbar^2}{2m_v^*} (k_\parallel^2 + k_z^2) = E_c^m + \frac{\hbar^2}{2m_c^*} (k_\parallel^2 + (k_z')^2) \]
\[ \implies \frac{\hbar^2}{2\mu} k_\parallel^2 + \frac{\hbar^2}{2m_v^*} k_z^2 + \frac{\hbar^2}{2m_c^*} (k_z')^2 = E_v^p - E_c^m = qV, \]
where \( \mu = m_c^* m_v^* / (m_c^* + m_v^*) \).

If we assume \( m_v^* = m_c^* = m^* = 2\mu \), we get the modified energy conservation relation:
\[ 2k_\parallel^2 + k_z^2 = \frac{2m^*}{\hbar^2} qV - (k_z')^2. \]

Denote \( \frac{2m^*}{\hbar^2} qV = k_{\max}^2 \). Now \((k_z')^2 \geq 0, \) and
\[ 2k_\parallel^2 + k_z^2 \leq k_{\max}^2 \]
is the surface bounding the volume of states in the \( k- \)space that contribute to tunneling current.

\[ J = \frac{2e}{qV} \sum_k v_g^z(k) T(k) [f_L(k) - f_R(k)]. \]

Spherical coordinates: \( k_z = k \cos \theta, \ k_\parallel = k \sin \theta. \)
Energy/momentum conservation volume \( \Omega: \)
\[ k_\parallel^2 \leq k_{\max}^2 / (1 + \sin^2 \theta). \] Then,
\[ J = \frac{2e}{(2\pi)^3} \int_\Omega d^3 k v_g^z(k) T(k) [f_L(k) - f_R(k)], \]
and we get:
\[ J = \frac{4m^*}{2\pi^2 \hbar^3} T_0 \bar{E}_\parallel \cdot [qV - 2\bar{E}_\parallel (1 - \exp[-qV/2\bar{E}_\parallel])]. \]

A part of the states in this hemisphere contribute to the tunnel current:

Tunnel current:

Reverse-bias

Debdeep Jena (djena@cornell.edu), Cornell University
**Tunneling Current: with lateral ‘k’ conservation**

\[
J = \frac{q m^*}{2\pi^2 \hbar^3} T_0 \vec{E}_|| \cdot \left[ qV - 2 \vec{E}_|| (1 - \exp[-qV/2\vec{E}_||]) \right].
\]

If \( qV \gg 2\hat{\vec{E}}_|| \),
\[ J \approx \frac{q^2 m^* T_0 \hat{\vec{E}}_||}{2\pi^2 \hbar^3} V \]
\[ \implies \sim \text{linear } I - V. \]

If \( qV \ll 2\hat{\vec{E}}_|| \),
\[ J \approx \frac{q^3 m^* T_0}{8\pi^2 \hbar^3} V^2 \]
\[ \implies \text{parabolic } I - V. \]

\[ T_0 = \exp\left[-\frac{\pi \sqrt{m^* E_g^{3/2}}}{2\sqrt{2}qF\hbar}\right] \]

\[ \vec{E}_|| = \frac{\sqrt{2}qF\hbar}{2\pi \sqrt{m^* E_g}} \]

Desired in: Ohmic contacts, Lasers, Solar Cells, TFETs, etc…

Desired in non-linear devices (backward diodes, etc)

Example: ~parabolic relation in GaN/AlN/GaN TJ (Simon, PRL 2009).
Tunneling Current: Forward & Reverse Bias

Kane’s general result:

\[ \frac{I}{A} = \frac{gm^*}{2\pi^2\hbar^3} P_0 \bar{\varepsilon} \times D \]

General form of DOS overlap

Kane (JAP 32 83 1961)
Simplest Case: A **Discrete** Two-Level System

\[ \hbar \delta \omega = \hbar \omega_{21} = (E_2 - E_1) + (W_{22} - W_{11}) \]

\[ i \hbar \frac{dc_2(t)}{dt} = c_1(t)e^{i\delta \omega t} W_{21} \]

\[ i \hbar \frac{dc_1(t)}{dt} = c_2(t)e^{-i\delta \omega t} W_{12} \]

Setting \( c_1(t) = b_1e^{i(\omega - \frac{1}{2}\delta \omega)t} \) and \( c_2(t) = b_2e^{i(\omega + \frac{1}{2}\delta \omega)t} \) to get

\[ b_1h(\omega - \frac{1}{2}\delta \omega) + b_2W_{21} = 0 \]

\[ b_1W_{12} + b_2h(\omega + \frac{1}{2}\delta \omega) = 0 \]

\[ |c_1(t)|^2 = 1 - C^2 \sin^2 \Omega t \]

\[ |c_2(t)|^2 = C^2 \sin^2 \Omega t \]

\[ C^2 = \frac{|W_{12}|^2}{(\frac{1}{2} \hbar \delta \omega)^2 + |W_{12}|^2} \]

\[ \omega = \pm \Omega = \pm \sqrt{|W_{12}|^2 + \left(\frac{1}{2} \delta \omega\right)^2} \]

\[ \omega = \pm \Omega = \pm \sqrt{|W_{12}|^2 + \left(\frac{1}{2} \delta \omega\right)^2} \]
Free-electron Hamiltonian in the presence of an electric field:
\[ \hat{H} = \frac{\hbar^2}{2m_0} \hat{k}_x^2 - eFx \]
where \( \hat{k}_x = -i\frac{\partial}{\partial x} \).

The expectation value of the operator \( \hat{k}_x(t) \) is (Ehrenfest’s theorem):
\[ \frac{d\langle \hat{k}_x \rangle}{dt} = -\frac{i}{\hbar} \left[ \hat{k}_x, \hat{H} \right] = -\frac{i}{\hbar} \left[ \hat{k}_x, -eFx \right] = \frac{ieF}{\hbar} \left[ \hat{k}_x, x \right] = -eF \]

\[ \Rightarrow \text{Force} = \hbar \frac{dk(t)}{dt} : \text{Newton’s law of motion in } k\text{-space} \]

Thus, the electric field sweeps electrons to \( |k\rangle \) states according to:
\[ k_x(t) = k_x(0) - eFt/\hbar \]

Allowed ‘nearly free-electron’ Energy Bands (time dependent for \( F \neq 0 \)):
- ‘CB’: \( E_0(k_x) = \frac{\hbar^2 k_x^2(t)}{2m_0} \)
- ‘VB’: \( E_1(k_x) = \frac{\hbar^2 (k_x(t)-G)^2}{2m_0} \)

The problem is analogous to a two-state system with:
→ The crystal potential as a time-independent perturbation, and
→ Force by electric field as a time-dependent perturbation.

Historical approach to understand tunneling (Oppenheimer, Zener, Landau):
As a time-dependent transition from one band to another.
Let $a_0(t)$ and $a_1(t)$: amplitudes of the electrons in bands $|k\rangle$ and $|k-G\rangle$ respectively.

Then, Schrödinger's equation for the 2-state system is:

$$i\hbar \frac{d}{dt} \begin{bmatrix} a_0(t) \\ a_1(t) \end{bmatrix} = \begin{bmatrix} E_0[k_x(t)] & -V_g \\ -V_g & E_0[k_x(t) - G] \end{bmatrix} \begin{bmatrix} a_0(t) \\ a_1(t) \end{bmatrix}$$

Solve these to find $a_0(t), a_1(t)$ - (if you can!) and you are done.

If the electron starts in band $|k\rangle$ and stays in it $\implies$ Tunneling.
If the electron transitions from band $|k\rangle \rightarrow |k-G\rangle \implies$ Bloch oscillation.

Thus, the tunneling probability is: $\implies T = \lim_{t \rightarrow \infty} |a_0(t)|^2$

Zener & Landau solved the eqns in 1932 and got:

The Landau-Zener formula: $T = \exp[-2\pi \Gamma]$, where $\Gamma = V_g^2 / \hbar \alpha$, and $\alpha = \frac{\partial (E_1 - E_0)}{\partial t} = \frac{\hbar G e F}{m_0}$

Thus, in the 2-band model, using the effective mass $\frac{m_0}{\hbar G} \approx \sqrt{\frac{m^*}{2E_g}}$,

$$T = \exp\left[-\frac{m_0 a E_g^2}{4\hbar^2 e F}\right] = \exp\left[-\frac{\pi}{2^{3/2}} \cdot \frac{\sqrt{m^* E_g^{3/2}}}{\hbar e F}\right]$$
**Interband tunneling in semiconductors**

Free electron vs. real bandstructure

Let $a_0(t)$ and $a_1(t)$: amplitudes of the electrons in bands $|k_i\rangle$ and $|k\rangle_G$ respectively. Then, Schrodinger's equation for the 2-state system is:

$$i\hbar \frac{d}{dt}\begin{bmatrix} a_0(t) \\ a_1(t) \end{bmatrix} = \sqrt{E_0}|k_x(t)\rangle - V_g V_g E_0 |k_x(t)\rangle_G.$$ 

Solve these to find $a_0(t)$, $a_1(t)$ - (if you can!) and you are done.

If the electron starts in band $|k_i\rangle$ and stays in it = Tunneling.

If the electron transitions from band $|k_i\rangle$ to $|k\rangle_G$ = Bloch oscillation.

Thus, the tunneling probability is:

$$T = \lim_{t \to \infty} |a_0(t)|^2.$$ 

Zener & Landau solved the eqns in 1932 and got: The Landau-Zener formula:

$$T = \exp\left[-\frac{m_0 a E_g^2}{4\hbar^2 e F}\right] = \exp\left[-\frac{\pi}{2^{3/2}} \frac{\sqrt{m^* E_g^{3/2}}}{\hbar e F}\right].$$

Use the right $m^*$ and $E_g$ and you’ll be ok 😊
Electrons tunnel through a barrier that is
• thin,
• small, or
• a combination

Tunneling could be interband or within the same band (intraband).

Impact ionization occurs for
• narrow bandgap semiconductors,
• heavily doped semiconductors, or
• a combination

Impact ionization occurs by carrier multiplication.
Tunneling in Semiconductors

Zener (Interband) Tunneling

bulk semiconductor  p-n junctions  heterojunctions
Classical Transistors:

Barrier-limited transport:
Subthreshold slope limit:
\((kT/q)\ln(10)\approx 60\, mV/\text{dec.}\)

How can we get steeper Sub-threshold slopes?

Measurements of 32 nm node CMOS \(n\) and \(p\) MOSFETs
The Tunneling Field-Effect Transistor (TFET)

Attributes:
1. normally-off,
2. saturated $I_{ON}$,
3. low $I_{OFF}$,
4. low $V_{DD}$,
5. subthreshold swing <60 mV/decade,
6. complementary

Slide from: Dr. Seabaugh
Graphene Tunnel-FETs

- GNRs capable of high tunneling currents
- Stems from thin body & no lateral momentum
- TFET approach: ‘Scale $E_g$ up from 0 eV’
- The ‘planar’ version of CNT FETs pioneered by Appenzeller et al, IBM.

- APL 93 112106 (2008)
- EDL 29 1344 (2008)
The Tunneling Field-Effect Transistor (TFET)

Figures from: Dr. Seabaugh

$J = \frac{I_D}{w} = \frac{q^3 t_{CH} V_R \sqrt{2m^*}}{8\pi^2 \hbar^2 \sqrt{E_G}} \xi \exp\left(-\frac{4\sqrt{2m^* E_G^3}}{3q\hbar \xi}\right)$

High tunnel currents favor narrow bandgap, low-mass materials

Low bandgap materials have higher tunneling probability

150 meV broken gap

114/xx
**A 2D crystal semiconductor p-n junction**

- **Problem:** Find the interband tunneling current in a 2D crystal semiconductor p-n junction

- **Current:**

\[
I_T = q \frac{g_s g_v}{L_x} \sum_k v_g(k) (f_v - f_c) T_{WKB}
\]

\[
T_{WKB} = \exp \left[ -\frac{4\sqrt{2m^*_R(E_g + E_y)^{3/2}}}{3q\hbar F} \right] \approx T_0 \exp \left[ -\frac{E_y}{\bar{E}} \right]
\]

\[
T_0 = \exp \left[ -4\sqrt{2m^*_R E_g^{3/2}} / 3q\hbar F \right]
\]

\[
\bar{E} = q\hbar F / 2\sqrt{2m^*_R E_g}
\]

\[
m_R^* = m_c^* m_v^* / (m_c^* + m_v^*)
\]

N. Ma and D. Jena

Debdeep Jena (djena@cornell.edu), Cornell University
Tunneling current in 2D crystal p-n junction

Estimates of interband tunneling currents in 2D crystal p-n junctions. Note the dependence on the electric field, bandgaps, and effective masses. The current can be boosted with electric fields.

N. Ma and D. Jena

Appl. Phys. Lett. 102, 132102 (2013)
Interlayer 2D Crystal Tunneling FETs

Challenges:
• Doping & contacts
• Stacking of 2D layers
• Device processing: contact alignment

Solutions:
• Modulation and chemical doping (+Prof. Chowalla’s method!)
• Direct van der Waal’s epitaxy
• Selective laser etching, patterned growth

Approach for achieving high on-currents: interlayer tunneling

In-plane TFETs

Interlayer TFETs

Tunneling Transistors Based on Graphene and 2-D Crystals

By Debdeep Jena, Member IEEE
SymFETs: Exploiting and controlling symmetry

SymFET: A Proposed Symmetric Graphene Tunneling Field-Effect Transistor
Pei Zhao, Student Member, IEEE, Randall M. Feenstra, Gong Gu, and Debdeep Jena

Geim/Novoselov/Eaves groups

- Predicted
- Measured

Resonant tunnelling and negative differential conductance in graphene transistors
L. Britnell¹, R. V. Gorbachev², A. K. Geim¹², L. A. Ponomarenko¹, A. Mishchenko¹,
M. T. Greenaway³, T. M. Fromhold³, K. S. Novoselov⁴ & L. Eaves¹³

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²Manchester Centre for Mesoscience & Nanotechnology, University of Manchester, Manchester M13 9PL, UK
³School of Physics & Astronomy, University of Nottingham, Nottingham NG7 2RD, UK
Decades of tunneling currents…

Esaki diode is still a radio star, half a century on

An FM transistor radio owned by one of us (L. E.) since the early 1960s still works beautifully. Reasoning that this was testament to the performance of its single Esaki diode, we tested the effects of storage on some of these germanium devices made in 1960.

The Esaki diode (L. Esaki Phys. Rev. 109, 603–604; 1958) was the first quantum-electron device. Unlike the mechanism that powers most semiconductor devices, current flows through the diode as a result of quantum-mechanical electron tunnelling across a potential barrier.

Semiconductor transport devices are extremely stable, so their shelf-life should be infinite if they are stored at room temperature. But the Esaki diode’s tunnel current is very sensitive to its enormous built-in electric field in the junction region (E. Spenke Electronic Semiconductors 232; McGraw-Hill, 1958), which could affect its long-term performance.

As the most likely indicator of any small structural changes in the device, we re-measured the peak current in 20 devices and discovered that it had fallen by an average of just 3.3% over 50 years, corresponding to a junction widening of only 0.25%.

This very tiny shift in electronic characteristics is probably down to inbuilt impurities and imperfections within the structure. A gratifying confirmation of the diode’s longevity, nonetheless.

Leo Esaki The Science and Technology Promotion Foundation of Ibaraki, Tsukuba 305-0032, and Yokohama College of Pharmacy, Japan e-mail: leoesaki@epochal.or.jp
Yasuhiro Arakawa, Masatoshi Kitamura Institute for Nano Quantum Information Electronics, The University of Tokyo, Komaba, Meguro 153-8505, Japan

And decades more to come!!

Debdeep Jena (djena@cornell.edu), Cornell University
Outline

Part I: Review of fundamentals

1: Review of classical and quantum mechanics
2: Current flow in quantum mechanics
3: Quantum statistics, quest for equilibrium as the driver for transport

Part II: Single-particle transport

4: Ballistic transport: Quantized conductance, Ballistic MOSFETs
5: Transmission and tunneling, Tunneling FETs
6. Closed vs. open systems, the Non-Equilibrium Green’s Function approach to transport
7. Diffusive transport: Boltzmann transport equation, scattering, electron-phonon interactions
8. High-field effects, Gunn diodes and oscillators for high-frequency power

Part III: Many-particle correlated transport

9: Fock-space way of thinking transport, second quantization, conductance anomalies
10: BCS theory of superconductivity, Josephson junctions
11. Landau/Ginzburg theories of phase transitions due to broken symmetry

Part III: Geometrical and topological quantum mechanics, unification with relativity

12: Spin, transport in a magnetic field, Quantum Hall effect, Berry phase in quantum mech
13: Chern numbers, Edge/Topological states, Topological insulators and Majorana Fermions
Scattering rate: \( W_{ij} = \frac{2\pi}{\hbar} |V_{ij}|^2 \delta(E_i - E_j) \), where states \( |i\rangle \) belong to the left electrode, states \( |j\rangle \) belong to the right electrode.

\[
I_{L\rightarrow R} = (-e) \sum_{i \in L, j \in R} W_{ij} f(E_i - \mu_L) \left[ 1 - f(E_j - \mu_R) \right]
\]

\[
I_{R\rightarrow L} = (-e) \sum_{i \in L, j \in R} W_{ij} f(E_j - \mu_R) \left[ 1 - f(E_i - \mu_L) \right]
\]

\[
I_{\text{tot}} = \frac{2\pi e}{\hbar} \sum_{i \in L, j \in R} |V_{ij}|^2 \left[ f(E_j - \mu_R) - f(E_i - \mu_L) \right] \delta(E_i - E_j)
\]

Introduce the density of states of the electrodes as

\[
n_L(E) = \sum_{i \in L} \delta(E - E_i)
\]

\[
n_R(E) = \sum_{j \in R} \delta(E - E_j)
\]

we get

\[
\int dE \sum_{i \in L, j \in R} \delta(E - E_i) \delta(E - E_j) = \delta(E_i - E_j)
\]

\[
I_{\text{tot}} = \frac{2\pi e}{\hbar} \int |V(E)|^2 \left[ f(E - \mu_R) - f(E - \mu_L) \right] n_L(E) n_R(E) dE
\]

\[
f(E) = \frac{1}{1 + \exp \left( \frac{E}{kT} \right)}
\]
Coherent Transport in Nanostructures

\[ W_{ij} = 2 |V_{ij}|^2 (E_i - E_j), \]

where states \( |i\rangle \) belong to the left electrode and states \( |j\rangle \) belong to the right electrode.

\[ I_{L} - I_{R} = (e) P \sum_{i,j} W_{ij} f(E_i - \mu_L) [1 - f(E_j - \mu_R)] \]

\[ I_{R} - I_{L} = (e) P \sum_{i,j} W_{ij} [f(E_j - \mu_R) - f(E_i - \mu_L)] \]

\[ I_{tot} = \frac{2\pi e}{\hbar} \int |V(E)|^2 [f(E - \mu_R) - f(E - \mu_L)] n_L(E) n_R(E) dE \]

\[ V(E) \propto \exp \left( -d \sqrt{\frac{2m(E_B - E)}{\hbar^2}} \right) \]

If there are no states in the ‘insulator’ or the ‘device’

The scattering matrix element will be shown (Bardeen - PRL 6 57 1961) to be related to **tunneling** from the left to the right electrode.

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Transport through a “single atomic state”

\[W_L = \frac{2\pi}{\hbar} |V_{i0}|^2 \delta(E_i - E_0) = \frac{\Gamma_L(E_0)}{\hbar}\]
\[W_R = \frac{2\pi}{\hbar} |V_{0j}|^2 \delta(E_0 - E_j) = \frac{\Gamma_R(E_0)}{\hbar}\]
\[I_{L\rightarrow|0\rangle} = -eW_L[f(E_0 - \mu_L) - f_0]\]
\[I_{|0\rangle\rightarrow R} = -eW_R[f_0 - f(E_0 - \mu_R)]\]
\[I_{L\rightarrow|0\rangle} = I_{|0\rangle\rightarrow R}\]

\[\implies f_0 = \frac{\Gamma_L(E_0)f(E_0 - \mu_L) + \Gamma_R(E_0)f(E_0 - \mu_R)}{\Gamma_L(E_0) + \Gamma_R(E_0)}\]

\[\implies I = \frac{e}{\hbar} [f(E_0 - \mu_R) - f(E_0 - \mu_L)] \frac{\Gamma_L(E_0)\Gamma_R(E_0)}{\Gamma_L(E_0) + \Gamma_R(E_0)}\]

If...
\[f(E_0 - \mu_R) - f(E_0 - \mu_L) \approx 1 \& \Gamma_L(E_0) = \Gamma_R(E_0) = \Gamma\]

\[\implies I = \frac{e\Gamma}{2\hbar}\]

\[\implies \text{We can draw as much current as we want by increasing the coupling with the electrodes. This is not consistent with experimental observations, which show a maximum possible conductance! Where is the catch?}\]
The ‘catch’: The discrete energy $E_0$ broadens due to coupling with the electrodes, similar to the FWHM in transitions in Fermi’s Golden Rule, and the linewidth of spontaneous emission.

\[
\delta(E - E_0) \rightarrow D(E) = \frac{\Gamma/2\pi}{(\Gamma/2)^2 + (E-E_0)^2}, \text{ where } \Gamma = \Gamma_L + \Gamma_R.
\]

\[
\Rightarrow I = \frac{e}{\hbar} [f(E_0 - \mu_R) - f(E_0 - \mu_L)] \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \text{ should be changed to }
\]

\[
I = \frac{e}{\hbar} \int_{-\infty}^{+\infty} dE D(E)[f(E_0 - \mu_R) - f(E_0 - \mu_L)] \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}
\]

For low temperatures, $f(E_0 - \mu_R) - f(E_0 - \mu_L) \approx 1$ for $\mu_R < E_0 < \mu_L$ and zero outside,
\[
\mu_L - \mu_R = eV_D,
\]

\[
\int \frac{\Gamma/2\pi}{(\Gamma/2)^2 + (E-E_0)^2} dE = \frac{1}{\pi} \tan^{-1} \left( \frac{E-E_0}{\Gamma/2} \right) \rightarrow
\]

\[
I = \frac{e}{\pi \hbar} \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \left[ \tan^{-1} \left( \frac{\mu_L - E_0}{\Gamma/2} \right) - \tan^{-1} \left( \frac{\mu_R - E_0}{\Gamma/2} \right) \right]
\]

Show that this leads to a maximum conductance $G_{\text{max}} = I/V_D = e^2/h$.
Broadening of the sharp channel eigenvalues due to strong coupling to contact eigenstates is the central ‘new’ feature. Variables get replaced by matrices for book-keeping convenience in dealing with interactions between discrete channel and contact states (or we will have a ton of coupled Schrodinger equations!).

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Dynamics of an open system

\[
\frac{dN}{dt} = -\left(\frac{\gamma_1 + \gamma_2}{\hbar}\right)N + \left(s_1 + s_2\right) \tag{43.6}
\]

Steady state:

\[
N = \frac{s_1 + s_2}{(\gamma_1 + \gamma_2)/\hbar} \tag{43.7}
\]

If no right contact ($s_2 = \gamma_2 = 0$), $N = f_1 = \frac{h s_1}{\gamma_1}$, implying $s_1 = \frac{\gamma_1}{\hbar} f_1$ and $s_2 = \frac{\gamma_2}{\hbar} f_2$. So

\[
N = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \tag{43.8}
\]

and the steady state current is

\[
I = q(s_1 - \frac{\gamma_1}{\hbar} N) = \frac{q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2) \tag{43.9}
\]
Dynamics of an open quantum system

Quantum version of this is obtained by going to $N(t) = \Psi \Psi^*$. Bound states $i\hbar \frac{d\Psi}{dt} = E\Psi$ yields $\frac{dN(t)}{dt} = \frac{d\Psi\Psi^*}{dt} = 0$. Modify Schrodinger equation for the open system...

Introduce an imaginary part of energy to let the state decay... $\Psi(t) = \psi(x)e^{-\frac{i}{\hbar}E_0t} \rightarrow \psi(x)e^{-\frac{i}{\hbar}E_0t}e^{-\frac{\gamma}{2\hbar}t}$. Here $E_0$ is the eigenvalue of the isolated system, which forms a state of definite energy and is isolated and bound. Without the source term,

$$\frac{d\Psi\Psi^*}{dt} = -\frac{\gamma}{\hbar} \Psi \Psi^* \quad (43.10)$$

which allows for the decay of the particle number now.
Dynamics of an open quantum system

Modified time-independent Schrodinger equation taking \(i\hbar \frac{d}{dt} \rightarrow E\) and adding source term now to fill the state (note we write \(\psi = \psi(x)\) as time-independent),

\[
E\psi = (E_0 - i\frac{\gamma}{2})\psi + (S_1 + S_2)
\]  

(43.11)

from where we obtain the wavefunction amplitude as

\[
\psi = \frac{S_1 + S_2}{(E - E_0) + i\frac{\gamma}{2}} \quad \Rightarrow \quad \psi\psi^* = \frac{S_1 S_1^* + S_2 S_2^* + S_1 S_2^* + S_2 S_1^*}{(E - E_0)^2 + (\frac{\gamma}{2})^2}
\]  

(43.12)

Interference terms will cancel: \(S_1 S_2^* + S_2 S_1^* = 0\). Then, if \(N\) denotes the steady state value of \(N(t)\), we get

\[
N = \int_{-\infty}^{\infty} dE \psi \psi^* = \int_{-\infty}^{\infty} dE \frac{S_1 S_1^* + S_2 S_2^*}{(E - E_0)^2 + (\frac{\gamma}{2})^2} \quad \leftrightarrow \quad N = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}
\]  

(43.13)
Net current through an open quantum system

Again we make the connection \( S_1 S_1^* = \gamma_1 f_1(E) \) and \( S_2 S_2^* = \gamma_2 f_2(E) \), and relate

\[
\mathcal{N} = \gamma_1 \int_{-\infty}^{\infty} \frac{dE f_1(E)}{(E - E_0)^2 + (\gamma/2)^2} + \gamma_2 \int_{-\infty}^{\infty} \frac{dE f_2(E)}{(E - E_0)^2 + (\gamma/2)^2} \leftrightarrow N = \frac{\gamma_1}{\gamma} f_1 + \frac{\gamma_2}{\gamma} f_2 \tag{43.14}
\]

Again \( \gamma = \gamma_1 + \gamma_2 \). And by analogy obtain the net current flowing out of terminal 1 as

\[
I = q\frac{\gamma_1}{\hbar} (f_1 - N) \leftrightarrow q\frac{\gamma_1}{\hbar} \left[ \gamma \int_{-\infty}^{\infty} dE \frac{f_1(E)}{(E - E_0)^2 + (\gamma/2)^2} - \mathcal{N} \right] \tag{43.15}
\]

which results in the quantum version of the current:

\[
I = \frac{q}{\hbar \gamma_1 \gamma_2} \int_{-\infty}^{\infty} \frac{dE}{(E - E_0)^2 + (\gamma/2)^2} [f_1(E) - f_2(E)] \leftrightarrow I = \frac{q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2) \tag{43.16}
\]
Net current through a quantum system

We have $\int_{-\infty}^{\infty} \frac{dE}{(E-E_0)^2 + (\frac{\gamma}{2})^2} = \frac{2\pi}{\gamma}$. For low temperatures, the values of the factor $f_1(E) - f_2(E) = 1$ for $\mu_2 \leq E \leq \mu_1$, where $\mu_1 - \mu_2 = qV$. The current then is

$$I = \frac{q}{\hbar} \gamma_1 \gamma_2 \int_{\mu_2}^{\mu_2 + qV} \frac{dE}{(E-E_0)^2 + (\frac{\gamma}{2})^2} = \frac{q}{\hbar} \frac{2\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \left[ \tan^{-1} \left( \frac{2(E_0 - \mu_2)}{\gamma} \right) - \tan^{-1} \left( \frac{2(E_0 - \mu_2 - qV)}{\gamma} \right) \right]$$

(43.17)
\[ |\Psi\rangle = \sum_n a_n |n\rangle \]

\[
\begin{bmatrix}
  a_1 \\
  a_2 \\
  a_3 \\
  \vdots
\end{bmatrix}
= 
\begin{bmatrix}
  \langle 1|\Psi\rangle \\
  \langle 2|\Psi\rangle \\
  \langle 3|\Psi\rangle \\
  \vdots
\end{bmatrix}
\]

\[ \langle \Psi | = \begin{bmatrix} a_1^* & a_2^* & a_3^* & \cdots \end{bmatrix} \]

\[ \langle \Psi|\Psi\rangle = 1 \quad \sum_n |a_n|^2 = 1 \]
\[ \hat{H} |n\rangle = E_n |n\rangle \quad |\Psi\rangle = \sum_n a_n |n\rangle \]
\[ \hat{H} |\Psi\rangle = E |\Psi\rangle \]
\[ \hat{H} \sum_n a_n |n\rangle = E \sum_n a_n |n\rangle \]
\[ \sum_n \langle m | \hat{H} |n\rangle a_n = E a_m \]

\[
\begin{align*}
H_{11} a_1 + H_{12} a_2 + H_{13} a_3 \ldots &= E a_1 \\
H_{21} a_1 + H_{22} a_2 + H_{23} a_3 \ldots &= E a_2 \\
H_{31} a_1 + H_{32} a_2 + H_{33} a_3 \ldots &= E a_3 \\
\vdots &= \vdots
\end{align*}
\]
\[ \begin{bmatrix}
H_{11} & H_{12} & H_{13} & \ldots \\
H_{21} & H_{22} & H_{23} & \ldots \\
H_{31} & H_{32} & H_{33} & \ldots \\
\vdots & \vdots & \vdots & \ddots
\end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix} = E \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix} \]
\[ \hat{H} \sum_n a_n |n\rangle = E \sum_n a_n |n\rangle \]

\[
\begin{bmatrix}
H_{11} & H_{12} & H_{13} & \cdots \\
H_{21} & H_{22} & H_{23} & \cdots \\
H_{31} & H_{32} & H_{33} & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{bmatrix}
\begin{bmatrix}
a_1 \\
a_2 \\
a_3 \\
\vdots
\end{bmatrix}
= E
\begin{bmatrix}
a_1 \\
a_2 \\
a_3 \\
\vdots
\end{bmatrix}
\]

\[ E a_n = E_0 a_n - t_0 a_{n-1} - t_0 a_{n+1} \]

\[ a_n = e^{ikx_n} \text{ gives } E = E_0 - t_0(e^{ika} + e^{-ika}) \]

which gives the bandstructure

\[ E(k) = E_0 - 2t_0 \cos(ka) \]
\[
E \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} E_0 & -t_0 \\ -t_0 & E_0 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} + \begin{bmatrix} -t_0 e^{-ika} & 0 \\ 0 & -t_0 e^{-ika} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} + \begin{bmatrix} A(1 - e^{2ika}) \\ 0 \end{bmatrix}
\]

or, in a compact form,

\[
E[\psi] = [H][\psi] + [\Sigma][\psi] + [s]
\]

\[
\begin{array}{c}
\Rightarrow \\
[\psi] = \left(EI - [H] - [\Sigma]\right)^{-1}[s] \Rightarrow [\psi] = [G(E)][s]
\end{array}
\]
An important ‘detail’: Self-consistency of potential

The charge in the channel ‘N’ and the electrostatic potential ‘U=−q∗V’ in the channel are linked, and need to be determined self-consistently.
**NEGF Matrices: Definitions**

The Green's function $G$ is defined as:

$$G = (EI - H - \Sigma)^{-1}$$

The source matrix $s$ is given by:

$$s = G \psi$$

The broadening matrix $\Sigma$ is the sum of the contact broadening matrices $\Sigma_1$ and $\Sigma_2$:

$$\Sigma = \Sigma_1 + \Sigma_2$$

The inverse of $G$ is:

$$G^{-1} = EI - H - \Sigma$$
NEGF Matrices: Definitions

\[ \psi = \left( EI - H - \Sigma \right)^{-1} G s = G s \]

\[ G = \left( EI - H - \Sigma \right)^{-1} \]

\[ G^{-1} = EI - H - \Sigma \]

Since \( H^\dagger = H \),

\[ (G^{-1})^\dagger - G^{-1} = \Sigma - \Sigma^\dagger \]

\[ [G^{-1}]^\dagger = EI - H - \Sigma^\dagger \]

Since \([G^{-1}]^\dagger = [G^\dagger]^{-1}\),

\[ G^\dagger = \left( EI - H - \Sigma^\dagger \right)^{-1} \]
NEGF Matrices: Definitions

The correlation function $G^n$ is the most important quantity is analogous to the carrier density. It is obtained by adding the $\psi\psi^\dagger$ contributions from all sources (contacts), and NOT $\psi$'s because different contacts inject carriers that are incoherent with no phase relationships. Note that $\psi^\dagger\psi$ is a NUMBER, whereas $\psi\psi^\dagger$ is a MATRIX. The number forgets phase information, the matrix remembers it. The correlation function preserves the phase of the injected electrons and any interferences within the device are thus included in the calculation. Also note that the correlation function consists in it information about the device through $H$, the contacts through $\Sigma$, as well as the battery through $f_1, f_2$. Thus it is an ‘all-knowing’ function (or matrix) and plays a central role in the device analysis. We just have to know what to ask of it!
\[ \Gamma_1 = i(\Sigma_1 - \Sigma_1^\dagger) \text{ and } \Gamma_2 = i(\Sigma_2 - \Sigma_2^\dagger) \]

\[ \Gamma = \Gamma_1 + \Gamma_2 \]

\[ \Gamma = i(\Sigma - \Sigma^\dagger) \text{ Self Energy} \]

\[ \Sigma^{in} = 2\pi s s^\dagger = \Gamma_1 f_1 + \Gamma_2 f_2 \text{ Source Injection Matrix} \]
**NEGF Matrices: Definitions**

\[ \Sigma^{in} = 2\pi ss^\dagger = \Gamma_1 f_1 + \Gamma_2 f_2 \]

*Source Injection Matrix*

\[ G^n = 2\pi \psi \psi^\dagger = 2\pi (G s)(s^\dagger \psi^\dagger) = G \Sigma^{in} G^\dagger \]

*Correlation function*

\[ G^n = G \Sigma^{in} G^\dagger \]

*Correlation function*

\[ A = i(G - G^\dagger) \]

*Spectral Function*
\[ \tilde{I}_{op}(E) = q \frac{d}{dt} \psi \psi^\dagger \]
\[ i\hbar \frac{d}{dt} (\psi \psi^\dagger) = (i\hbar \frac{d\psi}{dt}) \psi^\dagger + \psi (i\hbar \frac{d\psi^\dagger}{dt}) \]
\[ i\hbar \frac{d}{dt} \psi = H \psi + \Sigma \psi + s \]
\[ -i\hbar \frac{d}{dt} \psi^\dagger = \psi^\dagger H + \psi^\dagger \Sigma^\dagger + s^\dagger \]
\[ \tilde{I}_{op}(E) = \frac{q}{i\hbar} \text{Tr}[(i\hbar \frac{d\psi}{dt}) \psi^\dagger + \psi (i\hbar \frac{d\psi^\dagger}{dt})] \]
\[ \tilde{I}_{op}(E) = \frac{q}{i\hbar} \text{Tr}[ (H\psi\psi^\dagger - \psi\psi^\dagger H) + (\Sigma\psi\psi^\dagger - \psi\psi^\dagger \Sigma^\dagger) + (ss^\dagger G^\dagger - Gss^\dagger) ] \]

We identify \( 2\pi\psi\psi^\dagger = G^n \) and \( 2\pi ss^\dagger = \Sigma^{in} \) to write

\[ \tilde{I}_{op}(E) = \frac{q}{i\hbar} \text{Tr}[ \left( \frac{HG^n - G^n H}{2\pi} \right) + \left( \frac{\Sigma G^n - G^n \Sigma^\dagger}{2\pi} \right) + \left( \frac{\Sigma^{in} G^\dagger - G\Sigma^{in}}{2\pi} \right) ] \]

\[ \tilde{I}_{op}(E) = \frac{q}{i\hbar} \text{Tr}[ (HG^n - G^n H) + (\Sigma G^n - G^n \Sigma^\dagger) + (\Sigma^{in} G^\dagger - G\Sigma^{in}) ] \]
The Trace of matrices $A$ and $B$ has the property $\text{Tr}[AB] = \text{Tr}[BA]$, that is, the matrix products are allowed to commute inside the Trace operator. We can switch them around. Using this property, we realize that

$$\frac{q}{i\hbar} \text{Tr}[HG^n - G^n H] = 0 \quad (44.33)$$

The second term with $\Sigma G^n$ gives

$$\frac{q}{i\hbar} \text{Tr}[\Sigma G^n - G^n \Sigma^\dagger] = \frac{q}{i\hbar} \text{Tr}[(\Sigma - \Sigma^\dagger)G^n] = -\frac{q}{\hbar} \text{Tr}[\Gamma G^n] \quad (44.34)$$

where we again use $\text{Tr}[G^n \Sigma^\dagger] = \text{Tr}[\Sigma^\dagger G^n]$, and the definition $\Gamma = i(\Sigma - \Sigma^\dagger)$.

The last term gives

$$\frac{q}{i\hbar} \text{Tr}[\Sigma^{\text{in}} G^\dagger - G \Sigma^{\text{in}}] = \frac{q}{i\hbar} \text{Tr}[\Sigma^{\text{in}} (G^\dagger - G)] = \frac{q}{\hbar} \text{Tr}[\Sigma^{\text{in}} A] \quad (44.35)$$
NEGF method: Electric Current

\[ \tilde{I}_{op}(E) = \frac{q}{h} \text{Tr}[\Sigma^{in} A - \Gamma G^n] \]

\[ \tilde{I}_{op}^m(E) = \frac{q}{h} \text{Tr}[\Gamma_m(f_mA - G^n)] \]

\[ \tilde{I}_{op}^1(E) = \frac{q}{h} \text{Tr}[\Gamma_1 G \Gamma_2 G^\dagger] \times (f_1 - f_2) \]

\[ I_1 = \int_{-\infty}^{+\infty} dE \cdot \tilde{I}_{op}^1(E) = \frac{q}{h} \int_{-\infty}^{+\infty} dE \cdot \text{Tr}[\Gamma_1 G \Gamma_2 G^\dagger] \times \left[ f_1(E) - f_2(E) \right] \]
Example of Green’s Function Transport

\[
G(E) = \frac{1}{E - (E_{\text{f}} + W_{\text{b}}) - 2t_o e^{i\kappa a}} = \frac{1}{-W_o - 2i t_o \sin k a}
\]

\[E = E_{\text{f}} - 2t_o \sin k a\]

\[\mathcal{D}(E) = -\frac{\text{Tr}[A(E)]}{2\pi} = \frac{i}{2\pi} \left( \frac{\rho(E) - \rho_{\text{f}}}{\rho(E)} \right)
\]

(Density of states)

\[
\rho(E) = \frac{i}{2\pi} \frac{4t_o^2 \sin k a}{W_o^2 - 4t_o^2 \sin^2 k a} = \frac{2}{2\pi} \frac{t_o^2 \sin k a}{H_o^2 \sin k a - W_o^2}
\]

Transmision:

\[T_1 = i (\mathcal{E}_1 - \mathcal{E}_1^+) = i (t_o e^{i\kappa a} + t_o e^{i\kappa a}) = 2t_o \sin k a\]

\[T_2 = 2t_o \sin k a\]

\[T(E) = \text{Tr} (T_1 \rho(E) T_2^+) = \left( \frac{2t_o \sin k a}{W_o^2} \right)^2 \frac{1}{W_o^2 + (2t_o \sin k a)^2}
\]

Use \(E_{\text{f}} = E_{\text{f}} - 2t_o \sin k a\) to write in terms of energy \(E\).

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Single state $\rightarrow$ many states in the channel

Broadening of the sharp channel eigenvalues due to strong coupling to contact eigenstates is the central ‘new’ feature. Variables get replaced by matrices for book-keeping convenience in dealing with interactions between discrete channel and contact states (or we will have a ton of coupled Schrodinger equations!).
Charge current using Green’s Functions

Formal development of Green’s function technique

\[ I = \left( \frac{dQ_R}{dt} \right)_0 \]

\[ Q_R = \sum_{j \in R} (-e) \langle j | \rho | j \rangle \]

\[ \frac{d\rho}{dt} = \frac{1}{i\hbar} [H_0, \rho] + \frac{1}{i\hbar} [V, \rho] \]

\[ \rho_+ = \sum_{i \in L} |i_+\rangle f(\varepsilon_i - \mu_L) \langle i_+| \]

Density matrix

\[ I^+ = \frac{(-e)}{i\hbar} \sum_{j \in R} \langle j | [V, \rho_+] | j \rangle \]

\[ I^+ = \frac{(-e)}{i\hbar} \sum_{j \in R} \langle j | [V, \rho_+] | j \rangle \]

\[ I^+ = \frac{(-e)}{i\hbar} \sum_{j \in R, i \in L} \{ \langle j | t(\varepsilon_i) | i \rangle \langle i | V G^+(\varepsilon_i) | j \rangle - \text{c.c.} \} f(\varepsilon_i - \mu_L) \]

\[ t(\varepsilon) = V + VG(\varepsilon)V . \]

Note that ‘t’ retains the perturbation to an arbitrary order. 1st term: Fermi’s Golden Rule approximation.

\[ G^+_0(\varepsilon_i) | j \rangle = \frac{|j\rangle}{\varepsilon_i - \varepsilon_j - i\eta} \]

\[ \langle i | V G^+(\varepsilon_i) | j \rangle = \frac{\langle i | t^+(\varepsilon_i) | j \rangle}{\varepsilon_i - \varepsilon_j - i\eta} \]

\[ I^+ = \frac{2\pi(-e)}{\hbar} \sum_{i \in L, j \in R} |\langle j | t(\varepsilon_i) | i \rangle|^2 f(\varepsilon_i - \mu_L) \delta(\varepsilon_i - \varepsilon_j) \]

\[ \lim_{\eta \to 0^+} \left[ \frac{1}{x-i\eta} - \frac{1}{x+i\eta} \right] = i(2\pi) \delta(x) \]

\[ I^+ = \frac{2\pi(-e)}{\hbar} \sum_{i \in L, j \in R} |\langle j | t(\varepsilon_i) | i \rangle|^2 f(\varepsilon_i - \mu_L) \delta(\varepsilon_i - \varepsilon_j) \]

Current as a function of ‘transmission’ term ‘t’. Weak perturbation approximates \( t = V + VG_0V + VG_0VG_0V + \ldots \) by \( t \sim V \).

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Charge current using Green’s Functions

Let’s assume no direct transitions from the source electrode states $|i\rangle$ to the drain electrode states $|j\rangle$, i.e., $\langle i|V|j\rangle = 0$. This is valid when we neglect direct source $\rightarrow$ drain tunneling. This approximation can be removed if necessary.

\[
t = V + VG_0V + VG_0VG_0V + ...
\]

\[
t_{ij} = \langle i|t|j\rangle = \sum_{n,m} V_{in}G_{nm}V_{mj}
\]

\[
|t_{ij}|^2 = \sum_{n,m,n',m'} V_{in}G_{nm}V_{mj}V_{n'i}G_{n'm'}^{+}V_{jm'}
\]

\[
\Gamma_{nm}^{L}(\varepsilon) = 2\pi \sum_{i\in L} V_{ni}V_{im}\delta(\varepsilon - \varepsilon_i)
\]

\[
\Gamma_{nm}^{R}(\varepsilon) = 2\pi \sum_{j\in R} V_{nj}V_{jm}\delta(\varepsilon - \varepsilon_j)
\]

\[
I = \frac{e}{h} \int \sum_{n,n',m,m'} \Gamma_{n'n'}^{L}(\varepsilon)\Gamma_{nm}^{R}(\varepsilon)G_{nm}(\varepsilon)G_{nm'}^{+}(\varepsilon) \{ f(\varepsilon - \mu_R) - f(\varepsilon - \mu_L) \} \, d\varepsilon.
\]

\[
= \frac{e}{h} \int \text{Tr} \left[ I^{L}G^{R}G^{+} \right] \{ f(\varepsilon - \mu_R) - f(\varepsilon - \mu_L) \} \, d\varepsilon.
\]

\[
I = \frac{e}{h} \int T(\varepsilon) \{ f(\varepsilon - \mu_R) - f(\varepsilon - \mu_L) \} \, d\varepsilon.
\]

which is a generalization of the Landauer formula that relates the current to the transmission coefficient $T(\varepsilon) = \text{Tr} \left[ I^{L}G^{R}G^{+} \right]$ across the nano-device.
Current using Green’s Functions: Calculation method

Matrix realization of Green’s function procedure

\[
\begin{bmatrix}
[H_0]_{00} & [V]_{0L} & [V]_{0R} \\
[V]_{L0} & [H_0]_{LL} & 0 \\
[V]_{R0} & 0 & [H_0]_{RR}
\end{bmatrix}
\]

(8.51)

where the labels 0, L, R refer to the nano-device, the left and right reservoirs, respectively. Using (8.26), we have \((\eta \to 0^+)\)

\[
[G] = \begin{bmatrix}
(\varepsilon + i\eta) [I]_{00} - [H_0]_{00} & -[V]_{0L} & -[V]_{0R} \\
-[V]_{L0} & (\varepsilon + i\eta) [I]_{LL} - [H_0]_{LL} & 0 \\
-[V]_{R0} & 0 & (\varepsilon + i\eta) [I]_{RR} - [H_0]_{RR}
\end{bmatrix}^{-1}
\]

(8.52)

where \([I]\) is the unit matrix. We only need the nano-device part \([G]_{00}\) which, after straightforward algebra based on the Dyson’s equation (8.31), is given by

\[
[G]_{00} = \{(\varepsilon + i\eta) [I]_{00} - [H_0]_{00} - [\Sigma]\}^{-1}
\]

where

\[
[\Sigma] = [V]_{0R} [G_0]_{RR} [V]_{R0} + [V]_{0L} [G_0]_{LL} [V]_{L0}
\]

and

\[
[G_0]_{RR} = \{(\varepsilon + i\eta) [I]_{RR} - [H_0]_{RR}\}^{-1}
\]

\[
[G_0]_{LL} = \{(\varepsilon + i\eta) [I]_{LL} - [H_0]_{LL}\}^{-1}
\]

**$H_0 + V$ (perturbed Hamiltonian)**

**Green’s function matrix**

**Device Green’s function**

**Find the transmission**

**Get the current**

**Coupling matrices**
Old example: Transport through a single level

A Nano-Device with a Single Level. In order to discuss the physical meaning of the self-energy, we consider once again the case of a nano-device represented by a discrete and non-degenerate level of energy $\varepsilon_0$. The current is given by (8.49) with $n.m.n'.m' = 0$ and

$$G_{00}(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_0 - A(\varepsilon) + i[\Gamma(\varepsilon)/2]} .$$  \hspace{1cm} (8.58)

where $(\Gamma_{00}^{L} \equiv \Gamma^{L}, \Gamma_{00}^{R} \equiv \Gamma^{R})$

$$\Gamma(\varepsilon) = \Gamma^{L}(\varepsilon) + \Gamma^{R}(\varepsilon) . \quad A(\varepsilon) = \text{Re}(\Sigma_{00}) .$$  \hspace{1cm} (8.59)

Now we assume for simplicity that $\Gamma^{L}(\varepsilon), \Gamma^{R}(\varepsilon), \Gamma(\varepsilon)$ and $A(\varepsilon)$ are constant in the energy range where $f(\varepsilon - \mu_{R}) - f(\varepsilon - \mu_{L})$ is significant. Thus the current is given by the Landauer formula (8.50) with

$$T(\varepsilon) = \frac{\Gamma^{L} \Gamma^{R}}{\Gamma^{L} + \Gamma^{R}} A(\varepsilon) .$$  \hspace{1cm} (8.60)

where the line-shape is given by the Breit–Wigner formula

$$A(\varepsilon) = \frac{\Gamma}{(\varepsilon - \varepsilon_0 - A)^2 + (\Gamma/2)^2} .$$  \hspace{1cm} (8.61)

When $kT \ll \Gamma$, (8.50) leads to an analytic expression for the current through the single level

$$I = \frac{e}{h} \frac{\Gamma^{L} \Gamma^{R}}{\Gamma^{L} + \Gamma^{R}} \int_{\mu_{L}}^{\mu_{R}} A(\varepsilon) d\varepsilon ,$$

$$= \frac{2e}{h} \frac{\Gamma^{L} \Gamma^{R}}{\Gamma^{L} + \Gamma^{R}} \left[ \arctan \left( \frac{\mu_{R} - \varepsilon_0 - A}{\Gamma/2} \right) - \arctan \left( \frac{\mu_{L} - \varepsilon_0 - A}{\Gamma/2} \right) \right] .$$  \hspace{1cm} (8.62)

We recover the same result derived earlier for coherent transport through a single energy state.
NEGF on a two-level system
\[ H_{tot} = H_0 + W \]
\[ E\psi = H_0\psi + \Sigma \psi + s + W\psi \]
\[ \Sigma^{in} = 2\pi SS^\dagger = 2\pi (s + W\psi)(s^\dagger + \psi^\dagger W^\dagger) \]
\[ = 2\pi ss^\dagger + 2\pi W\psi\psi^\dagger W^\dagger + 2\pi (W\psi s^\dagger + s\psi^\dagger W^\dagger) \]
\[ = \Sigma_0^{in} + 2\pi W\psi\psi^\dagger W^\dagger + WG\Sigma_0^{in} + \Sigma_0^{in} G^\dagger W^\dagger \]

“Fermi Golden Rule”

interference → cancel for incoherent scattering
Outline

Part I: Review of fundamentals

1: Review of classical and quantum mechanics
2: Current flow in quantum mechanics
3: Quantum statistics, quest for equilibrium as the driver for transport

Part II: Single-particle transport

4: Ballistic transport: Quantized conductance, Ballistic MOSFETs
5: Transmission and tunneling, Tunneling FETs
6. Closed vs. open systems, the Non-Equilibrium Green’s Function approach to transport
7. Diffusive transport: Boltzmann transport equation, scattering, electron-phonon interactions
8. High-field effects, Gunn diodes and oscillators for high-frequency power

Part III: Many-particle correlated transport

9: Fock-space way of thinking transport, second quantization, conductance anomalies
10: BCS theory of superconductivity, Josephson junctions
11. Landau/Ginzburg theories of phase transitions due to broken symmetry

Part III: Geometrical and topological quantum mechanics, unification with relativity

12: Spin, transport in a magnetic field, Quantum Hall effect, Berry phase in quantum mech
13: Chern numbers, Edge/Topological states, Topological insulators and Majorana Fermions
Example: Exactly solvable 2-state problem

Simplest case: A 2-level system with step perturbation

|1⟩ → |2⟩  
|---|---|

E1  

E2

What is the occupation of states at time t?

Perturbation: 

W(r,t)

Example: Electrons in an atom with electric field perturbation. W=eF, W_{12}=eF<|x|2>=eFx_{12}~eF, r is ~ the size of the atom. For F~1 MV/cm, r~0.1 nm, W_{12}~10 meV (small energy, sharp resonance).

\[ h\delta\omega = h\omega_{21} = (E_2 - E_1) + (W_{22} - W_{11}) \]

\[ i\hbar \frac{dc_2(t)}{dt} = c_1(t)e^{i\delta\omega t} W_{21} \]

\[ i\hbar \frac{dc_1(t)}{dt} = c_2(t)e^{-i\delta\omega t} W_{12} \]

\[ |c_1(t)|^2 = 1 - C^2 \sin^2 \Omega t \]

\[ |c_2(t)|^2 = C^2 \sin^2 \Omega t \]

\[ C^2 = \frac{|W_{12}|^2}{(\frac{1}{2}h\delta\omega)^2 + |W_{12}|^2} \]

\[ \omega = \pm \Omega = \pm \sqrt{\frac{|W_{12}|^2}{\hbar^2} + (\frac{1}{2} \delta\omega)^2} \]

Setting \( c_1(t) = b_1e^{i(\omega - \frac{1}{2}\delta\omega)t} \) and \( c_2(t) = b_2e^{i(\omega + \frac{1}{2}\delta\omega)t} \) to get

\[ b_1\hbar(\omega - \frac{1}{2}\delta\omega) + b_2W_{21} = 0 \]

\[ b_1W_{12} + b_2\hbar(\omega + \frac{1}{2}\delta\omega) = 0 \]
The idea behind “Scattering”

Continuous, all weights

Discrete, specific frequencies

“Bands” and “Gaps”

States mixed; extended states may not be allowed \(\rightarrow\) localization, but gaps still possible
**Time-dependent perturbation theory**

\[
i\hbar \frac{\partial}{\partial t} |\Psi_t\rangle = H_0 |\Psi_t\rangle \quad \Rightarrow \quad i\hbar \frac{\partial}{\partial t} |\Psi_t\rangle = [H_0 + \text{W}_t] |\Psi_t\rangle
\]

**Unperturbed problem**

**Time-dependent perturbation**

If the system was in an eigenstate \(|\Psi_{t_0}\rangle = |0\rangle\) of energy \(E_0\) at time \(t_0\), then the state at a future time differs from the initial state by a phase factor

\[
H_0 |\Psi_{t_0}\rangle = E_0 |\Psi_{t_0}\rangle \quad \Rightarrow \quad |\Psi_t\rangle = e^{-i \frac{E_0}{\hbar} (t-t_0)} |\Psi_{t_0}\rangle.
\]

**Perturbation transformation**

\[
|\Psi_t\rangle = e^{-i \frac{H_0}{\hbar} t} |\Psi(t)\rangle
\]

**H**\(\text{O}\) is the Hamiltonian operator

\[
i\hbar \left( -i \frac{1}{\hbar} H_0 e^{-i \frac{H_0 t}{\hbar}} |\Psi(t)\rangle + e^{-i \frac{H_0 t}{\hbar}} \frac{\partial}{\partial t} |\Psi(t)\rangle \right) = [H_0 + \text{W}_t] e^{-i \frac{H_0 t}{\hbar}} |\Psi(t)\rangle
\]

**Time-dependent evolution in the Interaction picture**

\[
i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = [e^{i \frac{H_0}{\hbar} t} \text{W}_t e^{-i \frac{H_0}{\hbar} t}] |\Psi(t)\rangle = \text{W}(t) |\Psi(t)\rangle
\]

**Starting point for time-dependent perturbation theory**

| \(\Psi(t)\rangle = |\Psi(t_0)\rangle \)

\[
i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \text{W}(t) |\Psi(t)\rangle
\]

\[
|\Psi(t)\rangle = |\Psi(t_0)\rangle + \frac{1}{i\hbar} \int_{t_0}^{t} dt' \text{W}(t') |\Psi(t')\rangle
\]

**Figure 24.1:** Schrödinger vs. Interaction pictures of time-evolution of quantum state.

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**Time-dependent perturbation theory**

\[
|\Psi(t)\rangle = |\Psi(t_0)\rangle + \frac{1}{i\hbar} \int_{t_0}^{t} dt' W(t') |\Psi(t')\rangle
\]

Starting point for time-dependent perturbation theory

\[
W(t) = e^{iH_0 t} W_t e^{-iH_0 t}
\]

Approximation: retain terms to 1\textsuperscript{st} order in perturbation \(W\)

Assume that the perturbation is turned on 'slowly'

\[
W_t = e^{\eta t} W, \quad \eta = 0^+, \text{ and } W = W(t)
\]

\[
\langle n | \Psi(t) \rangle \approx \frac{1}{i\hbar} \int_{t_0}^{t} dt' \left[ \langle n | e^{i\frac{H_0}{\hbar} t'} \right] e^{\eta t'} W \left[ e^{-i\frac{H_0}{\hbar} t'} | 0 \rangle \right] = \frac{\langle n | W | 0 \rangle}{i\hbar} \int_{t_0}^{t} dt' e^{i\left(\frac{E_n-E_0}{\hbar}\right)t'} e^{\eta t'}
\]

\[
\int_{t_0}^{t} dt' e^{i\left(\frac{E_n-E_0}{\hbar}\right)t'} e^{\eta t'} = \frac{e^{i\left(\frac{E_n-E_0}{\hbar}\right)t} e^{\eta t} - e^{i\left(\frac{E_n-E_0}{\hbar}\right)t_0} e^{\eta t_0}}{i \left(\frac{E_n-E_0}{\hbar}\right) + \eta} \xrightarrow{t_0 \to -\infty} i \left(\frac{E_n-E_0}{\hbar}\right) + \eta
\]

Probability that the system is in state \(n\) at time \(t\)

\[
|\langle n | \Psi(t) \rangle|^2 = |\langle n | \Psi(t) \rangle|^2 \approx |\langle n | W | 0 \rangle|^2 \frac{e^{2\eta t}}{(E_0 - E_n)^2 + (\hbar \eta)^2}
\]
Time-dependent perturbation theory

The probability of the state making a transition from $|0\rangle$ to $|n\rangle$ at time $t$ is

$$|\langle n|\Psi_t\rangle|^2 = |\langle n|\Psi(t)\rangle|^2 \approx |\langle n|W|0\rangle|^2 \frac{e^{2\eta t}}{(E_0 - E_n)^2 + (\hbar\eta)^2}.$$  

The rate of transitions from state $|0\rangle \rightarrow |n\rangle$ is

$$\frac{1}{\tau_{|0\rangle \rightarrow |n\rangle}} \approx \frac{d}{dt} |\langle n|\Psi(t)\rangle|^2 \approx |\langle n|W|0\rangle|^2 \left(\frac{2\eta}{(E_0 - E_n)^2 + (\hbar\eta)^2}\right) e^{2\eta t}.$$  

$$\lim_{\eta \to 0^+} \frac{2\eta}{x^2 + \eta^2} = \lim_{\eta \to 0^+} \frac{1}{i} \left[ \frac{1}{x - i\eta} - \frac{1}{x + i\eta} \right] = 2\pi \delta(x).$$  

$$\delta(ax) = \delta(x) / |a|$$  

$$\frac{1}{\tau_{|0\rangle \rightarrow |n\rangle}} \approx \frac{2\pi}{\hbar} |\langle n|W|0\rangle|^2 \delta(E_0 - E_n),$$

**Fermi's golden rule for time-varying potentials**

Perturbations oscillating in time

$$W_t = 2We^{\eta t} \cos(\omega t) = e^{\eta t}W(e^{i\omega t} + e^{-i\omega t})$$  

$$\langle n|\Psi(t)\rangle \approx \frac{\langle n|W|0\rangle}{\imath\hbar} \left( \int_0^t dt' e^{i\left(\frac{E_n - E_0 + \hbar\omega}{\hbar}\right)t'} + \int_0^t dt' e^{i\left(\frac{E_n - E_0 - \hbar\omega}{\hbar}\right)t'} \right).$$  

$$\frac{1}{\tau_{|0\rangle \rightarrow |n\rangle}} \approx \frac{2\pi}{\hbar} \times |\langle n|W|0\rangle|^2 \times \left[ \delta(E_0 - E_n + \hbar\omega) + \delta(E_0 - E_n - \hbar\omega) \right].$$

**Fermi's golden rule for oscillating potentials**

$$\theta(\omega) = \int_0^\infty dt e^{\imath\omega t} = \lim_{\eta \to 0^+} \int_0^\infty dt e^{\imath\eta t} e^{\imath\omega t}$$  

$$= \lim_{\eta \to 0^+} \frac{i}{\omega + i\eta} = \frac{i}{\omega^+}$$

Two useful results to be used extensively later!

$$\int_{-\infty}^{+\infty} d\omega \frac{f(\omega)}{\omega^+} = P\left[ \int_{-\infty}^{+\infty} d\omega \frac{f(\omega)}{\omega} \right] - i\pi f(0)$$

Here $P[\ldots]$ is the “principal part” of a function.
Higher order perturbation theory

\[
|\psi(t)\rangle = |0\rangle_{|\psi(t)\rangle^{(0)}} + \frac{1}{i\hbar} \int_{t_0}^{t} dt' V(t') |0\rangle_{|\psi(t)\rangle^{(1)}} + \frac{1}{(i\hbar)^2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' V(t') V(t'') |0\rangle_{|\psi(t)\rangle^{(2)}} \\
+ \frac{1}{(i\hbar)^3} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \int_{t_0}^{t''} dt''' V(t') V(t'') V(t''') |0\rangle_{|\psi(t)\rangle^{(3)}} + ...,
\]

\[
\Gamma_{0\rightarrow n} = \frac{2\pi}{\hbar} \left| \langle n | V | 0 \rangle + \sum_{m} \frac{\langle n | V | m \rangle \langle m | V | 0 \rangle}{\epsilon_0 - \epsilon_m + i\eta \hbar} + \sum_{k,l} \frac{\langle n | V | k \rangle \langle k | V | l \rangle \langle l | V | 0 \rangle}{(\epsilon_0 - \epsilon_k + 2i\eta \hbar)(\epsilon_0 - \epsilon_l + i\eta \hbar)} + ... \right|^2 \delta(\epsilon_0 - \epsilon_n)
\]

\[
G = \sum_{m} \frac{|m\rangle \langle m|}{\epsilon_0 - \epsilon_m + i\eta \hbar}
\]

\[
\Gamma_{0\rightarrow n} = \frac{2\pi}{\hbar} \left| \langle n | V + VGV + VGVGV + ... | 0 \rangle \right|^2 \delta(\epsilon_0 - \epsilon_n)
\]
Transport in the ‘Diffusive’ Limit

Fermi’s Golden Rule tells us that the scattering potential is the SUM of ALL the scatterers in the macroscopic crystal.

How do multiple scattering centers add up and contribute to the total scattering rate?

\[
\frac{1}{\tau_{kk'}} = \frac{2\pi}{\hbar} |V(q)|^2 \delta[E_{k'} - (E_k \pm \hbar\omega)]
\]

\[q = k - k'\]

\[V(q) = \langle k'|W(r)|k \rangle\]

\[
= \int_{V} \left[ \frac{e^{-ik' \cdot r}}{\sqrt{V}} u_k^*(r) \right] \times W(r) \times \left[ \frac{e^{+ik \cdot r}}{\sqrt{V}} u_k(r) \right] d^3r
\]

\[
= \int_{V} \left[ \frac{e^{i(k-k') \cdot r}}{V} \right] W(r) \times [u_k^*(r)u_k(r)] d^3r
\]

\[
\approx \left( \int_{V} e^{iQ \cdot r} W(r) \frac{d^3r}{V} \right) \times \left( \int_{\Omega} u_k^*(r)u_k(r) \frac{d^3r}{\Omega} \right)
\]

\[
V(q) \approx \int_{V} e^{iQ \cdot r} W(r) \frac{d^3r}{V}
\]

Fourier Transform of real-space scattering potential!
Scattering rate due to point scatterers

\[ W(r) = V_0 \delta(r) \]

\[ \langle k'| V_0 \delta(r) | k \rangle = \int d^3r \left( \frac{e^{-ik' \cdot r}}{\sqrt{V}} \right) V_0 \delta(r) \left( \frac{e^{+ik \cdot r}}{\sqrt{V}} \right) = \frac{V_0}{V} \]

\[ \frac{1}{\tau(|k\rangle \rightarrow |k'|\rangle)} = \frac{2\pi}{\hbar} \left( \frac{V_0}{V} \right)^2 \delta(E_k - E_{k'}) \]

\[ \frac{1}{\tau(|k\rangle)} = \sum_{k'} \frac{1}{\tau(|k\rangle \rightarrow |k'|\rangle)} = \frac{2\pi}{\hbar} \left( \frac{V_0}{V} \right)^2 \sum_{k'} \delta(E_k - E_{k'}) \underbrace{D(E_k)}_{D(E_k)} \]

\[ \frac{1}{\tau(E_k)} = \frac{2\pi}{\hbar} \left( \frac{V_0}{V} \right)^2 n_{sc} V \int \frac{d^3k'}{(2\pi)^3 \sqrt{V}} \delta(E_k - E_{k'}) = \frac{2\pi}{\hbar} V_0^2 n_{sc} g(E_k) \]
Scattering by many impurities

\[ W_{total}(\mathbf{r}) = W(\mathbf{r}) + W(\mathbf{r} - \mathbf{R}_1) + W(\mathbf{r} - \mathbf{R}_2) + \ldots \]

\[ V_0(\mathbf{q}) \approx \int_V e^{i\mathbf{q} \cdot \mathbf{r}} W(\mathbf{r}) \frac{d^3 \mathbf{r}}{V} \]

\[ V_{total}(\mathbf{q}) = V_0(\mathbf{q}) + \int_V e^{i\mathbf{q} \cdot \mathbf{r}} W(\mathbf{r} - \mathbf{R}_1) \frac{d^3 \mathbf{r}}{V} + \ldots \]

\[ V_{total}(\mathbf{q}) = V_0(\mathbf{q}) + V_0(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{R}_1} + V_0(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{R}_2} \ldots \]

\[ V_{total}(\mathbf{q}) = V_0(\mathbf{q}) [1 + e^{i\mathbf{q} \cdot \mathbf{R}_1} + e^{i\mathbf{q} \cdot \mathbf{R}_2} \ldots] \]

\[ |V_{total}(\mathbf{q})|^2 = |V_0(\mathbf{q})|^2 \left[ (1 + e^{i\mathbf{q} \cdot \mathbf{R}_1} + e^{i\mathbf{q} \cdot \mathbf{R}_2} \ldots) \times (1 + e^{-i\mathbf{q} \cdot \mathbf{R}_1} + e^{-i\mathbf{q} \cdot \mathbf{R}_2} \ldots) \right] \]

\[ \approx 0(RPA) \]

\[ \left| e^{i\mathbf{q} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} + e^{i\mathbf{q} \cdot (\mathbf{R}_1 - \mathbf{R}_3)} \ldots \right| \]

\[ |V_{total}(\mathbf{q})|^2 = N_{imp} |V_0(\mathbf{q})|^2 \]

\[ \frac{1}{\tau_{kk'}(total)} = \frac{2\pi}{\hbar} N_{imp} \times |V_0(\mathbf{q})|^2 \delta[E_{k'} - (E_k \pm \hbar \omega)] \]

Scattering rate is linearly proportional to impurity density in the dilute uncorrelated limit!

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The Boltzmann Transport Equation

**Figure 30.1:** Scattering term of Boltzmann transport equation depicting the inflow and outflow of the distribution function.

\[
f = f(x, k, t) = f(x - v dt, k - \frac{F}{\hbar} dt, t - dt) + (S_{in} - S_{out}) dt
\]
The Boltzmann Transport Equation

\[ f = f(x, k, t) = f(x - v dt, k - \frac{F}{\hbar} dt, t - dt) + (S_{in} - S_{out}) dt \]

\[ \frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{F}{\hbar} \frac{\partial f}{\partial k} = S_{in} - S_{out} \]

\[ \frac{\partial f}{\partial t} + v_k \cdot \nabla_r f + \frac{F}{\hbar} \cdot \nabla_k f = S_{in} - S_{out} \]

\[ S_{in} = S(k' \rightarrow k) f_{k'}(1 - f_k), \]

\[ S_{out} = S(k \rightarrow k') f_k(1 - f_{k'}). \]

\[ \frac{\partial f_k}{\partial t} + v_k \cdot \nabla_r f_k + \frac{F}{\hbar} \cdot \nabla_k f_k = \sum_{k'} [S(k' \rightarrow k) f_{k'}(1 - f_k) - S(k \rightarrow k') f_k(1 - f_{k'})]. \]

\[ \text{scattering term, } \dot{C} f_k \]
The Boltzmann Transport Equation

\[
\frac{\partial f_k}{\partial t} + \mathbf{v}_k \cdot \nabla_r f_k + \frac{\mathbf{F}}{\hbar} \cdot \nabla_k f_k = \sum_{k'} \left[ S(k' \to k) f_{k'}(1 - f_k) - S(k \to k') f_k(1 - f_{k'}) \right].
\]

scattering term, \( \hat{C} f_k \)

\[
S(k \to k') = \frac{2\pi}{\hbar} |W_{k',k}|^2 \delta(E_k - E_{k'} \pm \hbar \omega)
\]

\[
S(k' \to k) f_{0k'}(1 - f_{0k}) = S(k \to k') f_{0k}(1 - f_{0k'})
\]

\[
\frac{S(k' \to k)}{S(k \to k')} = \frac{1 - f_{0k'}}{f_{0k'}} \cdot \frac{f_{0k}}{1 - f_{0k}} = e^{\frac{E_{k'} - E_k}{kT}}
\]
The Boltzmann Transport Equation

The microscopic nature of the collision term is given by

$$\frac{\partial f(k)}{\partial t}_{\text{coll}} = \sum_{k'} [S(k', k)f(k') [1 - f(k)] - S(k, k')f(k) [1 - f(k')]].$$  \hspace{1cm} (85)$$

Figure 11: Scattering term of Boltzmann transport equation depicting the inflow and outflow of the distribution function.

At equilibrium ($f = f_0$), the ‘principle of detailed balance’ enforces the condition

$$S(k', k)f_0(k') [1 - f_0(k)] = S(k, k')f_0(k) [1 - f_0(k')],$$

which translates to

$$S(k', k)e^{\frac{E_k}{k_B T}} = S(k, k')e^{\frac{E_{k'}}{k_B T}}.$$  

In the special case of elastic scattering, $\varepsilon_k = \varepsilon_{k'}$, and as a result, $S(k', k) = S(k, k')$. 
Enforcing the principle of detailed balance is telling us that for electrons, the scattering rate from state $|k\rangle \rightarrow |k'\rangle$ is not the same as for the reverse process, unless the energies of the two states are the same. For elastic scattering events $E_k = E_{k'}$ for which the energy of the electron is unchanged, the scattering rate $S(k \rightarrow k') = S(k' \rightarrow k)$ is the same for a process and its reverse. But for inelastic scattering events with $E_{k'} - E_k = \hbar \omega$, the scattering rate going uphill in energy is slower: $S(k \rightarrow k') = S(k' \rightarrow k)e^{-\hbar \omega / kT}$. The scattering rates $S(\ldots)$ remain the same whether electrons are in equilibrium or not, the occupation functions $f$ are what change.

Consider for example, the electron scattering rate due to either the absorption or emission of phonons of energy $\hbar \omega$. The rate of phonon absorption must be proportional to the number of phonons already present, i.e., $S_{\text{abs}} \propto n_{\text{ph}}$. The rate of phonon emission by an electron requires it to go downhill in energy, thus $S_{\text{em}} = S_{\text{abs}} e^{\hbar \omega / kT} \propto e^{\hbar \omega / kT} n_{\text{ph}}$.

Since the number of phonons in mode $\omega$ is given by the Bose-Einstein function $n_{\text{ph}} = 1/(e^{\hbar \omega / kT} - 1)$, we note that $e^{\hbar \omega / kT} n_{\text{ph}} = 1 + n_{\text{ph}}$. Thus, $S_{\text{abs}} \propto n_{\text{ph}}$, but $S_{\text{em}} \propto (1 + n_{\text{ph}})$. Electrons are free to ‘emit’ phonons even when there are no phonons present - thus, the ‘1’ represents spontaneous emission. But if there already are phonons present, the emission rate is enhanced, or stimulated; this is the reason for the $1 + n_{\text{ph}}$ proportionality of the net emission rate.
The Collision Integral

\[ \hat{C}f_k = \sum_{k'} S(k \to k')(e^{\frac{E_{k'}-E_k}{kT}} f_{k'}(1-f_k) - f_k(1-f_{k'})) \]

\[ E_{k'} - E_k = \hbar \omega_0 >> kT \]

\[ f_k f_{k'} << f_k' \]

\[ \hat{C}f_k \approx e^{\frac{\hbar \omega_0}{kT}} \sum_{k'} S(k \to k') f_{k'} \]

\[ \hat{C}f_k = \sum_{k'} S(k \to k')(f_{k'} - f_k) = \sum_{k'} S(k \to k') f_{k'} - \frac{f_k}{\tau(k)} \]

Inelastic Scattering

Elastic Scattering
Quantum and Momentum Scattering Rates

\[ \frac{\partial f(k)}{\partial t} \bigg|_{coll} = \sum_{k'} S(k, k')(f(k') - f(k)). \]

One can rewrite this collision equation as

\[ \frac{df(k)}{dt} + \frac{f(k)}{\tau_q(k)} = \sum_{k'} S(k, k')f(k'), \]

where the quantum scattering time is defined as

\[ \frac{1}{\tau_q(k)} = \sum_{k'} S(k, k'). \]

quantum scattering rate (dephasing)

\[ f(k) = f_0(k) - \tau F_t \cdot v \frac{\partial f_0(k)}{\partial \varepsilon}. \]

\[ f(k') - f(k) = e\tau \frac{\partial f_0}{\partial \varepsilon} \frac{E \cdot v'}{f(k) - f_0(k)} \left(1 - \frac{E \cdot v'}{E \cdot v} \right) \]

\[ \frac{1}{\tau_m(k)} = \sum_{k'} S(k, k')(1 - \frac{E \cdot k'}{E \cdot k}) \]

momentum scattering rate (mobility, conductivity)

\[ \frac{1}{\tau_m(k)} = \sum_{k'} S(k, k')(1 - \cos \theta) \]

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The Fermi level and temperature at equilibrium

\[ \frac{\partial f_k}{\partial t} + \mathbf{v}_k \cdot \nabla_r f_k + \frac{F}{\hbar} \cdot \nabla_k f_k = \sum_{k'} \left[ S(k' \rightarrow k) f_{k'} (1 - f_k) - S(k \rightarrow k') f_k (1 - f_{k'}) \right]. \]

scattering term, \( \hat{C}_{f_k} \)

\[ \frac{\partial f_0}{\partial t} = 0 \text{ at equilibrium} \]

\[ \hat{C}_{f_0} = 0 \]

\[ \mathbf{v}_k \cdot \nabla_r f_0 + \frac{F}{\hbar} \cdot \nabla_k f_0 = 0 \]

\[ \frac{\partial f_0}{\partial \varepsilon} = \frac{\partial g}{\partial \varepsilon} \frac{\partial f_0}{\partial g} = - \frac{1}{kT} \frac{e^g}{(1+e^g)^2} \implies \frac{\partial f_0}{\partial g} = kT \frac{\partial f_0}{\partial \varepsilon} \]

\[ \nabla_r f_0 = kT \frac{\partial f_0}{\partial \varepsilon} \nabla_r g \text{ and } \nabla_k f_0 = kT \frac{\partial f_0}{\partial \varepsilon} \nabla_k g \]

\[ kT \cdot \frac{\partial f_0}{\partial \varepsilon} \cdot \mathbf{v}_k \cdot \left[ \frac{F}{kT} + \nabla_r g \right] = 0 \]

\[ \frac{\mathbf{F}}{kT} + \nabla_r g = 0 \text{ requires} \]

\[ \frac{1}{kT} \left( \mathbf{F} + \nabla_r E_c(r) - \nabla_r E_F(r) \right) + \left[ E_c(r) + \varepsilon_c(k) - E_F(r) \right] \nabla_r \left( \frac{1}{kT} \right) = 0. \]

since \( \mathbf{F} = -\nabla_r E_c(r) \)

\[ -\nabla_r E_F(r) + \left[ E_c(r) + \varepsilon_c(k) - E_F(r) \right] T \nabla_r \left( \frac{1}{T} \right) = 0. \]

would imply \( \nabla_r E_F(r) = 0 \) and \( \nabla_r T_L(r) = 0 \), implying the Fermi level and the lattice temperature are equal everywhere at equilibrium.

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The Boltzmann Transport Equation

\[ f_0(\varepsilon) = \frac{1}{1 + e^{\frac{\varepsilon - \mu}{k_B T}}} \]

The Boltzmann transport equation gives a full-blown treatment of transport properties, and can be solved in several levels of approximation.

**Particle number conserved**

**Relaxation time approximation**

**equilibrium**

**perturbation**

The Boltzmann Transport Equation

\[ \frac{df}{dt} = \frac{F_t}{\hbar} \cdot \nabla_k f(k) + \mathbf{v} \cdot \nabla_r f(k) + \frac{\partial f}{\partial t} \]

\[ \frac{\partial f}{\partial t} = \frac{\partial f}{\partial t} \bigg|_{\text{coll}} - \frac{F_t}{\hbar} \cdot \nabla_k f(k) - \mathbf{v} \cdot \nabla_r f(k) \]

\[ \frac{\partial f}{\partial t} \bigg|_{c} = \frac{-(f - f_0)}{\tau_m} \]

\[ f = f_0 - \frac{\tau_m}{\hbar} \nabla_k \mathcal{E} \cdot \left( \frac{\partial f}{\partial \mathcal{E}} \mathbf{F} + \nabla_r f \right) \]

**equilibrium**

**scattering**

**bandstructure**

**applied forces**

**conc. gradients**

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Many electrons: Model by Distribution Function

\[ n = \int \frac{d^d k}{(2\pi)^d} f(k) = \int d\varepsilon f(\varepsilon) g_d(\varepsilon) \]

\[ g_d(\varepsilon) = \frac{1}{2^{d-1}\pi^{d/2}} \frac{m^*}{\hbar^2} \frac{d}{2} \varepsilon^{d/2-1} \]

\[ J = 2e \int \frac{d^d k}{(2\pi)^d} \mathbf{v} f(k) \]

\[ J_i = en \left( -\frac{2e}{dm^*} \frac{\int d\varepsilon \tau_m \varepsilon^{d/2} \frac{\partial f_0}{\partial \varepsilon}}{\int d\varepsilon f_0(\varepsilon) \varepsilon^{d/2-1}} \right) F_i \]

\[ f(k) = f_0(k) + eF_i \tau(k) \frac{\partial f_0}{\partial \varepsilon} \]

**Basic ideas:**
- If we know the distribution function and the bandstructure, then the current can be calculated.
- The distribution function changes from the equilibrium Fermi-Dirac form in response to perturbation.

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The Boltzmann Transport Equation

Boltzmann equation →

\[ f(k) = f_0(k) + e\tau_m(k)(\mathbf{F} \cdot \mathbf{v}) \frac{\partial f_0(k)}{\partial \varepsilon} \]

\[ \frac{1}{\tau_m(k)} = \sum_{k'} S(k, k')(1 - \cos \theta) - \text{Momentum scattering time} \quad (\mu = \frac{e\langle \tau_m(k) \rangle}{m^*}) \]

\[ \frac{1}{\tau_q(k)} = \sum_{k'} S(k, k') - \text{Quantum scattering time} \]

\[ S(k, k') = \frac{2\pi}{\hbar} \left| \langle k' | \Delta E_c(r) | k \rangle \right|^2 \delta(\varepsilon_k - \varepsilon_{k'}) \]

Most general expression for ‘Current Density’ in ‘d’ dimensions:

\[ \mathbf{J}_d = q \times \frac{g_s g_v}{L_d} \sum_k \mathbf{v}_g(k) f(k) \]

where

charge current density (general case)

Fermi’s Golden Rule gives: Scattering rate from state \( k \to k' \) by perturbation \( \Delta E_c \)

\( q\mathbf{v}_g \) may be replaced by other physical quantities:

\( q\mathbf{v}_g \to \text{charge current density (electrical cond.)} \)

\( 1 \to \text{carrier density} \)

\( \mathbf{E}(k) \to \text{heat current density (thermal cond.)} \)

…
Scattering events in semiconductors

Scattering processes

- Elastic
  - Coulombic: Remote impurities, Background impurity, Charged dislocations, Strain field of dislocations, Dipoles in alloy
  - Isotropic: Alloy disorder, Interface roughness, Acoustic phonon

- Inelastic
  - Optical phonon

A static periodic potential causes no scattering \(\rightarrow\) every other potential causes scattering!

Periodic ‘non-static’ potentials: Phonons.
Static non-periodic potentials: Defects & Impurities.
Scattering events in semiconductors

Scattering processes

Elastic

Coulombic
Remote impurities
Background impurity
Charged dislocations
Strain field of dislocations
Dipoles in alloy

Isotropic
Alloy disorder
Interface roughness
Acoustic phonon

Inelastic
Optical phonon

Scattering by each type of impurity affects the net electron mobility.

- Mobility in a ultra-clean (defect-free) semiconductor is limited by phonon (optical+acoustic) scattering.
- If the scattering rate of defects/impurities exceed that of phonons, then they determine the mobility.
- Method: find the scattering rate due to each type of defect. The total scattering rate is the sum of all.
Calculating the mobility/conductivity

\[ f = f_0 + q\tau_m \frac{\partial f_0}{\partial \varepsilon} \mathbf{v} \cdot \mathbf{E} \]

\[ \langle v \rangle = \frac{\int_{-\infty}^{\infty} v f \, dv}{\int_{-\infty}^{\infty} f \, dv} \]

\[ \langle v \rangle = \frac{\int_{-\infty}^{\infty} v f_0 \, dv + q \int_{-\infty}^{\infty} \tau_m (\partial f_0 / \partial \varepsilon) v (\mathbf{v} \cdot \mathbf{E}) \, dv}{\int_{-\infty}^{\infty} f_0 \, dv + q \int_{-\infty}^{\infty} \tau_m (\partial f_0 / \partial \varepsilon) (\mathbf{v} \cdot \mathbf{E}) \, dv} \]

\[ \langle v \rangle = \frac{q \int_{-\infty}^{\infty} \tau_m (\partial f_0 / \partial \varepsilon) v (\mathbf{v} \cdot \mathbf{E}) \, dv}{\int_{-\infty}^{\infty} f_0 \, dv} \]

\[ v_{dx} = -\mu_c E_x \quad \mu_c = \frac{q \langle \tau_m \rangle}{m^*} \quad J_x = \frac{q^2 n \langle \tau_m \rangle}{m^*} E_x \quad \sigma = \frac{q^2 n \langle \tau_m \rangle}{m^*} \]

Thus, for the simple case of a small applied electric field, we can define all the transport parameters in terms of the average momentum relaxation time, \( \langle \tau_m \rangle \). Once \( \langle \tau_m \rangle \) has been obtained, the transport problem is solved.
Formalism for diffusive charge transport

- Find the perturbation potential due to the defect.
- Use Fermi’s Golden rule to evaluate the single-particle scattering rate
- Add up for all allowed states
- Use the solution of Boltzmann equation to find the mobility/conductivity.

\[ V(q) = \langle k'| W(r) | k \rangle \]

\[ \mathcal{E}_c(r) = \mathcal{E}_c^0 + W(r) \]

Fermi’s golden rule

\[ \frac{1}{\tau_{kk'}} = \frac{2\pi}{\hbar} |V(q)|^2 \delta[E_{k'} - (E_k \pm \hbar \omega)] \]

Distribution function: Solution of Boltzmann Transport Equation

\[ f(k) = f_0(k) + eF_i \tau(k) \frac{\partial f_0}{\partial \epsilon} \]

Current density: Sum over all group velocities \( \mathbf{v} \) in \( k \)-space

\[ J = 2e \int \frac{d^d k}{(2\pi)^d} \mathbf{v} f(k) \]
Scattering by a neutral impurity

\[ \mathcal{E}_c(r) = \mathcal{E}_c^0 + W(r) \]

\[ W(r) = W_0 \Theta(r - r_0) \]

\[ V(q) = \langle k' | W(r) | k \rangle \]

\[ \frac{1}{\tau_{kk'}} = \frac{2\pi}{\hbar} |V(q)|^2 \delta[E_{k'} - (E_k \pm \hbar \omega)] \]

\[ \langle \tau_m \rangle = \frac{2}{3} \frac{\int_0^\infty \tau_m(-\partial f_0/\partial x)x^{3/2} \, dx}{\int_0^\infty f_0 x^{1/2} \, dx} \]

\[ \mu_c = \frac{q \langle \tau_m \rangle}{m^*} \]

For example, for electrons in Ge, where \( m/m_0 = 0.12 \) and \( \chi = 16 \), a mobility of \( 1.1 \times 10^3 \text{ cm}^2/\text{Vs} \) is obtained assuming, e.g., \( 10^{17} \text{ cm}^{-3} \) neutral impurities.

This & next few slides: material from
- Wolfe/Holonyak/Stillman
- Seeger

From Seeger: Derive your own expression!
Scattering by charged impurities

Screened coulomb scattering potential

\[ V(r) = -\left(\frac{Ze}{4\pi\kappa_0 r}\right) \exp\left(-\frac{r}{L_D}\right) \]

\[ |k-k'| \approx 2k \sin(\theta/2) \]

\[ \beta_{BH} = 2\frac{m}{\hbar} \left(\frac{2}{3} k_B T\right)^{1/2} L_D \]

Brooks-Herring dimensionless factor

\[ \beta_{BH} = \left(\frac{\kappa}{16}\right)^{1/2} \frac{T}{100 K} \left(\frac{m}{m_0}\right)^{1/2} \left(2.08 \times 10^{18} \text{ cm}^{-3}\right)^{1/2} \]

\[ H_{kk} = -\frac{Ze^2}{V \kappa_0 |k-k'|} \int_0^\infty \exp\left(-\frac{r}{L_D}\right) \sin(|k-k'| r) \, dr \]

\[ = -\frac{Ze^2}{V \kappa_0} \frac{1}{|k-k'|^2 + L_D^2} \approx -\frac{Ze^2}{V \kappa_0 4k^2} \frac{1}{\sin^2(\theta/2) + (2k L_D)^{-2}} \quad (6.3.13) \]

The mobility \( \mu = (e/m) \langle \tau_m \rangle \) is given by

\[ \mu = \frac{2^{7/2}(4\pi \kappa_0)^2(k_B T)^{3/2}}{\pi^{3/2} Z^2 e^3 m^{1/2} N_1 \left[\ln(1 + \beta_{BH}^2) - \beta_{BH}^2/(1 + \beta_{BH}^2)\right]} \]

which in units of cm²/V s is

\[ \mu = \frac{3.68 \times 10^{20} \text{ cm}^{-3}}{N_1} \frac{1}{Z^2} \left(\frac{\kappa}{16}\right)^2 \left(\frac{T}{100 K}\right)^{1.5} \frac{1}{(m/m_0)^{1/2} \left[\ln(1 + \beta_{BH}^2) - 0.434 \beta_{BH}^2/(1 + \beta_{BH}^2)\right]} \]

and the log is to the base 10.

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**Phonons in Semiconductors**

Newton’s law for mass-spring chain

\[ F = M \frac{d^2 u_s}{dt^2} = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) \]

\[ u_s = u_0 e^{i(qs \alpha - \omega t)} \]

Vibrations form a wave

\[ \omega^2(q) = \frac{2C}{M} (1 - \cos qa) \]

Acoustic phonon dispersion
Phonons in Semiconductors

Acoustic and optical phonon dispersion

\[ \omega_{\pm}(k) = \frac{C}{M_r} \left[ 1 \pm \sqrt{1 - \frac{2M_r}{M_1 + M_2} (1 - \cos ka)} \right] \]
Phonons in Semiconductors

Typical phonon spectra of semiconductors

Difference in energies of longitudinal and optical acoustic phonons
Deformation Potential Acoustic Phonon Scattering Potential

\[ u(r, t) = au(r, t) \]  \hspace{1cm} (6.4)

where

\[ u(r, t) = u \exp \left[ i(q \cdot r - \omega t) \right] \]  \hspace{1cm} (6.5)

In these equations \( a \) is the displacement direction, and \( u \) is the amplitude. The strain associated with the displacement is

\[ \nabla \cdot u(r, t) = a \cdot \nabla u(r, t) \]  \hspace{1cm} (6.6)

\[ \nabla \cdot u(r, t) = i q \cdot a u(r, t) \]  \hspace{1cm} (6.7)

Equation (6.7) indicates that for the transverse components of a phonon where the displacement and the wavevector are orthogonal, \( q \cdot a = 0 \), and no strain is produced. The scattering potential for the longitudinal component is, therefore,

\[ \Delta U(r, t) = \xi_A \nabla \cdot u(r, t) \]  \hspace{1cm} (6.8)

where the deformation potential, \( \xi_A \), in units of energy, is defined as the proportionality constant between the scattering potential (units of energy) and the strain.

Figure 6.2  Displacements of a diatomic chain for LA and TA phonons at (a) the center and (b) the edge of the Brillouin zone. The lighter mass atoms are indicated by open circles. For zone edge acoustic phonons only the heavier atoms are displaced.
Electron-Piezoelectric Acoustic Phonon interaction

\[ \Delta U(r, t) = -q \psi(r, t) \]

\[ \psi(r, t) = - \int E(r, t) \cdot dr \]

\[ D(\omega) = \varepsilon(\omega)E = \varepsilon_0 E + P(\omega) \]

\[ D(0) = \varepsilon(0)E = \varepsilon_0 E + P(0) \]

\[ D(0) = \varepsilon(0)E(r, t) + e_{pz} \nabla u(r, t) \]

\[ E(r, t) = - \frac{e_{pz}}{\varepsilon(0)} \nabla u(r, t) \]

\[ \Delta U(r, t) = \frac{-q e_{pz}}{\varepsilon(0)} u(r, t) \]

\[ \Delta U(r, t) = \frac{i q e_{pz}}{\varepsilon(0) q_x} \nabla \cdot u(r, t) \]

Figure 6.2 Displacements of a diatomic chain for LA and TA phonons at (a) the center and (b) the edge of the Brillouin zone. The lighter mass atoms are indicated by open circles. For zone edge acoustic phonons only the heavier atoms are displaced.

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Piezoelectric Acoustic Phonon Scattering Potential

Piezo charge
Electron-Def. Pot. Optical Phonon interaction

Typical phonon spectra of semiconductors

Optical Deformation Potential scattering potential $D \sim 10^8$ eV/cm

Figure 6.3  Displacements of a diatomic chain for LO and TO phonons at (a) the center and (b) the edge of the Brillouin zone. The lighter mass atoms are indicated by open circles. For zone edge optical phonons only the lighter atoms are displaced.

\[
\delta u(r, t) = u_1(r, t) - u_2(r, t)
\]  

\[
\Delta U(r, t) = D \delta u(r, t)
\]  

where $u_1(r, t)$ and $u_2(r, t)$ have the form given by (6.4) and (6.5). The scattering potential due to modulation of the conduction and valence edges must then be proportional to this relative displacement and

\[
\delta u(r, t) = a \delta u(r, t)
\]
Electron-Polar Optical Phonon interaction

\[ D(0) = e(0)E = e_0E + P(0) \]

\[ D(\infty) = e(\infty)E = e_\infty E + P(\infty) \]

\[ P(0) = P(\infty) + P_i \]

Using (6.24) in (6.21) and subtracting (6.21), we obtain
\[ \epsilon(0)E = \epsilon(\infty)E + P_i \]

or
\[ D(0) = e(\infty)E + P_i \]

From (6.24) we can determine the internal fields induced by the optical phonon polarization of the unit cell.

The polarization of a unit cell, \( P_i(r, t) \), is determined by the relative displacement of the ions in a unit cell, \( \delta u(r, t) \), and the effective ionic charge, \( e^* \), such that
\[ P_i(r, t) = \frac{e^*}{\Omega} \delta u(r, t) \]

In this equation \( \Omega = V/N \) is the volume of the \( N \) primitive or Wigner–Seitz unit cells and \( e^* \) is the Born effective charge given by
\[ e^* = \Omega \omega_{LO} \epsilon(\infty) \rho^{1/2} \left[ \frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)} \right]^{1/2} \]

where \( \rho \) is the mass density. This equation is derived in Chapter 7. Assuming no space or surface charges, (6.24) and (6.25) give an internal field,

\[ E(r, t) = -\frac{e^*}{\Omega \epsilon(\infty)} \delta u(r, t) \]

\[ \epsilon_e(0) / \epsilon_e(\infty) = (\omega_{LO} / \omega_{TO})^2 \]

as the Lyddane–Sachs–Teller relation

Using (6.9), (6.10), and (6.26), the scattering potential for polar mode scattering is
\[ \Delta U(r, t) = -\frac{q e^*}{\Omega \epsilon(\infty)} \int \delta u(r, t) \cdot dr \] (6.27)

or with (6.5) and (6.19),
\[ \Delta U(r, t) = -\frac{i q e^*}{\Omega \epsilon(\infty) q_s} \delta u(r, t) \] (6.28)

A comparison of (6.18) and (6.28) shows that the scattering potentials for deformation potential and polar mode scattering by optical phonons are out of phase by 90° and are thus independent.

Frohlich interaction

Polar optical phonon scattering potential

Optical phonon absorption and emission processes

Debdeep Jena (djena@cornell.edu), Cornell University
Electron-Phonon Scattering Rates

**Polar optical phonon**

\[
D = \epsilon_0 E + \frac{q^* u}{\Omega} \\
E(x, t) = -\frac{q^* u}{\epsilon_0 \Omega} \\
W(r, t) = -q \int dx E(x, t) = \frac{q}{i \beta \epsilon_0} \cdot q^* \cdot u_0 e^{i(\beta r - \omega t)} \\
\left( \frac{q^*}{\Omega} \right)^2 = \rho c_0 \omega_0^2 \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_a^2} \right) \\
W(r, t) = -q \int dx E(x, t) = \frac{q\omega_0 \sqrt{\beta}}{i \beta} \sqrt{\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_a^2}} \cdot u_0 e^{i(\beta r - \omega t)}
\]

**Deformation potential acoustic phonon**

\[
W(x, t) = D_{ac} \frac{\partial u}{\partial x} \\
W(r, t) = D_{ac}(\nabla \cdot \mathbf{u}) = iD_{ac}\beta u_0 e^{i(\beta r - \omega t)}
\]

**Deformation potential optical phonon**

\[
W(r, t) = D_{op} u = D_{op} u_0 e^{i(\beta r - \omega t)}
\]

**Piezoelectric acoustic phonon**

\[
D = \epsilon_0 \varepsilon_\alpha E + \varepsilon_{ps} \frac{\partial u}{\partial x} \\
E(x, t) = -\frac{\varepsilon_{ps}}{\epsilon_0 \varepsilon_\alpha} \frac{\partial u}{\partial x} \\
W(r, t) = -q \int dx E(x, t) = \frac{q\varepsilon_{ps}}{\epsilon_0 \varepsilon_\alpha} u_0 e^{i(\beta r - \omega t)} \\
K^2 = \frac{\varepsilon_{ps}^2}{\epsilon_0 \varepsilon_\alpha v_\alpha}
\]

**Momentum conservation**

\( \hbar k' = \hbar k \pm \hbar \beta \)

**Energy conservation**

\( E_{k'} = E_k \pm \hbar \omega_\beta \)

**Allowed angles for acoustic phonon scattering events**

\( \beta = 2k(\mp \cos \theta \pm \frac{m^* v_\beta}{\hbar k}) = 2k(\mp \cos \theta \pm \frac{v_\beta}{v_k}) \)

**Allowed angles for optical phonon scattering events**

\( \beta = \mp k \cos \theta \pm \sqrt{k^2 \cos^2 \theta \pm \frac{2m^* \hbar \omega_\beta}{\hbar^2}} \)

For acoustic phonons, \( \hbar \omega_\beta = \hbar v_\alpha \beta \), and we get

For optical phonons, we get

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Phonons in Semiconductors

\[ u_s(x, t) = u_0 e^{i(\beta x - \omega t)} + u_0 e^{-i(\beta x - \omega t)} \]

\[ |u_s|^2 = 4u_0^2 \cos(\beta x - \omega t) \]

\[ KE = \frac{1}{2} M \left( \frac{du_s}{dt} \right)^2 = 2M\omega^2u_0^2 \sin^2(\beta x - \omega t) \]

\[ PE = \frac{1}{2} Ku_s^2 = 2Ku_0^2 \cos^2(\beta x - \omega t) \]

but... \[ \omega^2 = \frac{K}{M} \rightarrow \]

\[ KE + PE = 2M\omega^2u_0^2 = N_\omega \cdot \hbar \omega \rightarrow \]

since... \[ M = \rho V, \]

\[ u_0^2 = \frac{\hbar}{2\omega \rho V} \cdot N_\omega \]

\[ N_\omega(T) = \frac{1}{e^{\hbar \omega / kT} - 1} \]
Electron-Acoustic Phonon interaction: Mobility

\[ \delta r = A_i \exp [\pm i (q_i \cdot r)] \]
\[ |H_{k'k}| = \frac{\varepsilon_{ac} q_i A_i}{V} |\int \exp [i(k' - k + q_i) \cdot r] d^3r| \]
\[ k' = k \pm q_i \]
\[ |H_{kk'}| = \varepsilon_{ac} q_i A_i. \]

2 \( M \omega^2 u_0^2 \approx N_{ph} \times \hbar \omega \)

\[ N \rightarrow N_q = [\exp (\hbar \omega / k_B T) - 1]; \]
\[ |H_{k\pm q, k}| = \varepsilon_{ac} q_i [(N_q + 1/2 \mp 1/2) \hbar/2 qV \omega]^{1/2}. \]
\[ |H_{kk'}| = \varepsilon_{ac} q_i [k_B T/2 qV \omega]^2 = \varepsilon_{ac} [k_B T/2 V c_l]^{1/2}. \]

\[ c_l = \rho v_s^2 \]

SHO: \(|\text{amplitude}|^2 \sim \text{number of phonons} \]

\[ S \approx \frac{2 \pi}{\hbar} |H_{k'k}|^2 [\delta(\varepsilon(k') - \varepsilon(k) + \hbar \omega) + \delta(\varepsilon(k') - \varepsilon(k) - \hbar \omega)] \]
\[ \approx \frac{2 \pi}{\hbar} |H_{k'k}|^2 \delta (\varepsilon(k') - \varepsilon(k)). \]

Deformation potential

Piezoelectric

Coupling \( K \sim 10^{-3} \)

\[ \Delta U(r, t) = \varepsilon_A \nabla \cdot \mathbf{u}(r, t) \]
\[ \mu = \frac{2 \sqrt{2\pi}}{3} \frac{e \hbar^4 c_l}{m^{5/2} (k_B)^{3/2} \varepsilon_{ac}^2} T^{-3/2} \]
which in units of \( \text{cm}^2/\text{V s} \) is given by
\[ \mu = 3.06 \times 10^4 \frac{c_l/10^{12} \text{ dyn cm}^{-2}}{(m/m_0)^{5/2} (T/100 \text{ K})^{3/2} (e_{ac}/eV)^2} \propto T^{-3/2}. \]
Electron-Optical Phonon Scattering Rates, Mobility

Deformation potential Optical Phonon

$$\mu_0 = \frac{4 \sqrt{2\pi} e \hbar^2 Q(k_B \Theta)^{1/2}}{3 m^{5/2} D^2} f(T/\Theta)$$

The function $f(T/\Theta)$ is given by

$$f(T/\Theta) = (2z)^{5/2}(e^{2z} - 1) \int_0^\infty \frac{y^{3/2} e^{-2zy} dy}{\sqrt{y + 1 + e^{2z}} \text{Re} \{\sqrt{y - 1}\}},$$

where $z = \Theta/2T$ and $y = \epsilon/k_B \Theta$. The function is shown.

Its numerical value in units of cm$^2$/V s is given by

$$\mu = 2.04 \times 10^3 \frac{(\epsilon/g \text{ cm}^{-3})(\Theta/400 \text{ K})^{1/2}}{(m/m_0)^{5/2}(D/10^8 \text{ eV cm}^{-1})^2} f(T/\Theta)$$

Polar Optical Phonon Scattering

$$\alpha = \frac{\hbar |e| E_0}{2^{1/2} m^{1/2}(\hbar \omega_0)^{3/2}} = \frac{1}{137} \sqrt{\frac{m c^2}{2k_B \Theta}} \left(\frac{1}{\chi_{\text{opt}}} - \frac{1}{\chi}\right)$$

$$= 397.4 \sqrt{\frac{m/m_0}{\Theta/K}} \left(\frac{1}{\chi_{\text{opt}}} - \frac{1}{\chi}\right)$$

The mobility is simply $(e/m) \tau_m$:

$$\mu = \frac{|e|/(2m \alpha \omega_0)}{1} \exp(\Theta/T)$$

which in units of cm$^2$/V s is given by

$$\mu = 2.6 \times 10^5 \frac{\exp(\Theta/T)}{\alpha(m/m_0)(\Theta/K)}$$

for $T \ll \Theta$

For example, in n-type GaAs where $\Theta = 417 \text{ K}$, $m/m_0 = 0.072$, $\alpha = 0.067$, we calculate a mobility at 100 K of $2.2 \times 10^5 \text{ cm}^2/\text{V s}$. This is of the order of magnitude of the highest mobilities observed in this material.
### TABLE 6.1 Scattering Potentials and Matrix Elements for Various Scattering Mechanisms

<table>
<thead>
<tr>
<th>Scattering Mechanisms</th>
<th>Scattering Potential</th>
<th>Matrix Element</th>
</tr>
</thead>
<tbody>
<tr>
<td>Impurities</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ionized</td>
<td>$\frac{Zq^2}{4\pi\epsilon(0)r}$</td>
<td>$\frac{Zq^2}{\epsilon(0)V</td>
</tr>
<tr>
<td>Neutral</td>
<td>$\frac{\hbar^2}{m^<em>} \left(\frac{r_B}{r^</em>}\right)^{1/2}$</td>
<td>$\frac{2\pi\hbar^2}{m^*V} \left(\frac{20r_B}{k}\right)^{1/2}$</td>
</tr>
<tr>
<td>Acoustic phonons</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Deformation potential</td>
<td>$\bar{\epsilon}_A \nabla \cdot \textbf{u}$</td>
<td>$\bar{\epsilon}_A \left(\frac{\hbar}{2V\rho\omega_s}\right)^{1/2} (\textbf{a} \cdot \textbf{q}_s) \left(n_q + \frac{1}{2} \pm \frac{1}{2}\right)^{1/2}$</td>
</tr>
<tr>
<td>Piezoelectric</td>
<td>$\frac{iq\epsilon_{\text{p}z}}{\epsilon(0)q_s} \nabla \cdot \textbf{u}$</td>
<td>$\frac{q\epsilon_{\text{p}z}}{\epsilon(0)} \left(\frac{\hbar}{2V\rho\omega_s}\right)^{1/2} \left(n_q + \frac{1}{2} \pm \frac{1}{2}\right)^{1/2}$</td>
</tr>
<tr>
<td>Optical phonons</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Deformation potential</td>
<td>$D\delta u$</td>
<td>$D \left(\frac{\hbar}{2V\rho\omega_{\text{LO}}}\right)^{1/2} \left(n_q + \frac{1}{2} \pm \frac{1}{2}\right)^{1/2}$</td>
</tr>
<tr>
<td>Polar</td>
<td>$\frac{iq\epsilon^*}{\omega\epsilon(\infty)q_s} \delta u$</td>
<td>$\frac{q\epsilon^*}{\Omega\epsilon(\infty)q_s} \left(\frac{\hbar}{2V\rho\omega_{\text{LO}}}\right)^{1/2} \left(n_q + \frac{1}{2} \pm \frac{1}{2}\right)^{1/2}$</td>
</tr>
</tbody>
</table>

---

$^a$ $r_B =$ Bohr radius; $n_q =$ phonon occupation number; $\epsilon^* = \Omega\omega_{\text{LO}}\epsilon(\infty)\rho^{1/2}[1/\epsilon(\infty) - 1/\epsilon(0)]^{1/2}$.  

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### TABLE 6.2  
Momentum Relaxation Times and Reduced Energy Dependence for Materials with Isotropic Parabolic Bands

<table>
<thead>
<tr>
<th>Scattering Mechanisms</th>
<th>$\tau_i$ (sec)</th>
<th>$r_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Impurities</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ionized</td>
<td>$\frac{0.414\varepsilon_s^2(0)T^{3/2}}{Z^2N_A(cm^{-3})g(n^<em>, T, x)} \left(\frac{m^</em>}{m}\right)^{1/2}$</td>
<td>$\frac{2}{3}$</td>
</tr>
<tr>
<td>Neutral</td>
<td>$\frac{8.16 \times 10^6}{\varepsilon_s(0)N_A(cm^{-3})} \left(\frac{m^*}{m}\right)^2$</td>
<td>0</td>
</tr>
<tr>
<td><strong>Acoustic phonons</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Deformation potential</td>
<td>$\frac{2.40 \times 10^{-20}C_l(dyn/cm^2)}{\varepsilon_s^2(eV)T^{3/2}} \left(\frac{m}{m^*}\right)^{3/2}$</td>
<td>$-\frac{1}{3}$</td>
</tr>
<tr>
<td>Piezoelectric</td>
<td>$\frac{9.54 \times 10^{-8}}{h \gamma_4(V/cm)(3/C_l + 4/C_r)T^{1/2}} \left(\frac{m}{m^*}\right)^{1/2}$</td>
<td>$\frac{1}{3}$</td>
</tr>
<tr>
<td><strong>Optical phonons</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Deformation potential</td>
<td>$\frac{4.83 \times 10^{-20}C_l(dyn/cm^2)[\exp(\theta/T) - 1]}{\varepsilon_s^2(eV)T^{1/2}\theta} \left(\frac{m}{m^*}\right)^{3/2}$</td>
<td>$\equiv -\frac{1}{3}$</td>
</tr>
<tr>
<td>Polar</td>
<td>$\frac{9.61 \times 10^{-15}\varepsilon_s(0)\varepsilon_s(\infty)[\exp(\theta/T) - 1]}{[\varepsilon_s(0) - \varepsilon_s(\infty)]\theta^{1/2}(\theta/T)^r} \left(\frac{m}{m^*}\right)^{1/2}$</td>
<td>$r \left(\frac{\theta}{T}\right)$</td>
</tr>
</tbody>
</table>

---

\(N_I = \) concentration of ionized impurities; \(g(n^*, T, x) = \ln(1 + b) - b/(1 + b); b = 4.31 \times 10^{13}[\varepsilon_s(0)T^2/n^*(cm^{-3})](m^*/m)x; N_N = \) concentration of neutral impurities; \(C_l = \frac{1}{3}(3C_{11} + 2C_{12} + 4C_{44}); \) \(C_r = \frac{1}{3}(C_{11} - C_{12} + 3C_{44}); \theta = h\omega_{LO}/k.\)
# Material Properties relevant for Transport

## TABLE 6.3 Parameters for Calculating the Transport Properties of n-Type Semiconductors with Isotropic Parabolic Bands

<table>
<thead>
<tr>
<th>Material</th>
<th>$\frac{m^*}{m}$</th>
<th>$\epsilon_r(0)$</th>
<th>$\epsilon_r(\infty)$</th>
<th>$\theta$ (K)</th>
<th>$\varepsilon_A$ (eV)</th>
<th>$C_t$ ($10^{12}$ dyn/cm$^2$)</th>
<th>$\frac{h_4^2}{C_t} \left( \frac{3}{C_t} + \frac{4}{C_t} \right)$ ($10^3$ V$^2$/dyn)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>0.218</td>
<td>9.87</td>
<td>5.80</td>
<td>1044</td>
<td>8.4</td>
<td>2.65</td>
<td>18.32</td>
</tr>
<tr>
<td>GaP</td>
<td>0.13</td>
<td>11.10</td>
<td>9.11</td>
<td>580</td>
<td>13.0</td>
<td>1.66</td>
<td>1.15</td>
</tr>
<tr>
<td>GaAs</td>
<td>0.067</td>
<td>12.53</td>
<td>10.90</td>
<td>423</td>
<td>6.3</td>
<td>1.44</td>
<td>2.04</td>
</tr>
<tr>
<td>GaSb</td>
<td>0.042</td>
<td>15.69</td>
<td>14.44</td>
<td>346</td>
<td>8.3</td>
<td>1.04</td>
<td>0.192</td>
</tr>
<tr>
<td>InP</td>
<td>0.082</td>
<td>12.38</td>
<td>9.55</td>
<td>497</td>
<td>6.8</td>
<td>1.21</td>
<td>0.137</td>
</tr>
<tr>
<td>InAs</td>
<td>0.025</td>
<td>14.54</td>
<td>11.74</td>
<td>337</td>
<td>5.8</td>
<td>1.0</td>
<td>0.192</td>
</tr>
<tr>
<td>InSb</td>
<td>0.0125</td>
<td>17.64</td>
<td>15.75</td>
<td>274</td>
<td>7.2</td>
<td>0.79</td>
<td>0.409</td>
</tr>
<tr>
<td>ZnS</td>
<td>0.312</td>
<td>8.32</td>
<td>5.13</td>
<td>506</td>
<td>4.9</td>
<td>1.28</td>
<td>6.87</td>
</tr>
<tr>
<td>ZnSe</td>
<td>0.183</td>
<td>9.20</td>
<td>6.20</td>
<td>360</td>
<td>4.2</td>
<td>1.03</td>
<td>0.620</td>
</tr>
<tr>
<td>ZnTe</td>
<td>0.159</td>
<td>9.67</td>
<td>7.28</td>
<td>297</td>
<td>3.5</td>
<td>0.84</td>
<td>0.218</td>
</tr>
<tr>
<td>CdS</td>
<td>0.208</td>
<td>8.58</td>
<td>5.26</td>
<td>428</td>
<td>3.3</td>
<td>0.85</td>
<td>32.5</td>
</tr>
<tr>
<td>CdSe</td>
<td>0.130</td>
<td>9.40</td>
<td>6.10</td>
<td>303</td>
<td>3.7</td>
<td>0.74</td>
<td>16.7</td>
</tr>
<tr>
<td>CdTe</td>
<td>0.096</td>
<td>10.76</td>
<td>7.21</td>
<td>246</td>
<td>4.0</td>
<td>0.70</td>
<td>0.445</td>
</tr>
<tr>
<td>HgSe</td>
<td>0.0265</td>
<td>25.6</td>
<td>12.0</td>
<td>268</td>
<td>4</td>
<td>0.80</td>
<td>0.445</td>
</tr>
<tr>
<td>HgTe</td>
<td>0.0244</td>
<td>20.0</td>
<td>14.0</td>
<td>199</td>
<td>4</td>
<td>0.61</td>
<td>0.445</td>
</tr>
<tr>
<td>PbS</td>
<td>175</td>
<td>17</td>
<td></td>
<td>300</td>
<td>20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PbSe</td>
<td>250</td>
<td>24</td>
<td></td>
<td>190</td>
<td>24</td>
<td>0.71</td>
<td></td>
</tr>
<tr>
<td>PbTe</td>
<td>400</td>
<td>33</td>
<td></td>
<td>160</td>
<td>25</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Note relative Strengths!*
Scattering events in semiconductors

Scattering processes

Elastic

Inelastic

Coulombic

Remote impurities
Background impurity
Charged dislocations
Strain field of dislocations
Dipoles in alloy

Isotropic

Alloy disorder
Interface roughness
Acoustic phonon
Optical phonon

Scattering by each type of impurity affects the net electron mobility.

- Mobility in a ultra-clean (defect-free) semiconductor is limited by phonon (optical+acoustic) scattering.
- If the scattering rate of defects/impurities exceed that of phonons, then they determine the mobility.
- Method: find the scattering rate due to each type of defect. The total scattering rate is the sum of all.

Figure 6.7 Temperature dependence of the mobility for n-type GaAs showing the separate and combined scattering processes. [From C. M. Wolfe, G. E. Stillman, and W. T. Lindley, J. Appl. Phys. 41, 3088 (1970).]
Handling Diffusive Transport in Low-Dimensions

Example: Transport in 2DEGs

2DEG electron wavefunction (note: \( k, r \) are in the 2D plane!)

\[
\frac{1}{\sqrt{A}} e^{i k \cdot r} \chi(z) u_{nk}(r) \rightarrow S(k, k') = \frac{2\pi}{\hbar} |H_{k,k'}|^2 \delta(\varepsilon_k - \varepsilon_{k'})
\]

\[
H_{k,k'} = \langle k' | V(r, z) | k \rangle \cdot I_{k,k'}
\]

\[
1 - \cos \theta = q^2 / 2k_F^2
\]

In general, scattering can lead to intersubband transitions…

Screening in 2D

\[
\epsilon_{2d}(q) = \epsilon(0) (1 + \frac{q_{TF}}{q})
\]

2D screening function

\[
q_{TF} = \frac{m^* \epsilon^2}{2\pi \epsilon(0) \epsilon_0 \hbar^2} = \frac{2}{a_B^*}
\]

Thomas-Fermi wavevector

\[
V(q, z_0) = \frac{V_{uns}(q, z_0)}{\epsilon_{2d}(q)}
\]

Screened 2D potential

\[
V_{nm}(q) = \frac{1}{A} \int dz \left( \chi_n^*(z) \chi_m(z) \int d^2r V(r, z) e^{iqr} \right)
\]

\( n, m \) are the subband indices

Within the same subband: ‘Electric quantum limit’

\[
V(q) = V_{00}(q) = \frac{1}{A} F(q) V(q, z_0)
\]
Handling Diffusive Transport in Low-Dimensions

\[ \rho(z) \rightarrow e n_s \delta(z) \]

\[ \rho(r, z) = \rho(z) = e n_s |\chi(z)|^2 \]

\[ \chi_{n_z}(z) = \sqrt{\frac{2}{L_z}} \sin \left( \frac{n_z \pi}{L_z} z \right) \]

- 'perfect' 2D: Graphene, BN
- Quasi-2D: MOSFETs/HEMTs
- 'Infinitely' deep square QW

- Triangular QW: Variational Wavefunction (Fang-Howard)
- Can handle multiple subband occupation…

\[ \chi(z) = \begin{cases} 
0, & z < 0 \\
\sqrt{\frac{b^3}{2}} e^{-\frac{b z}{2}}, & z \geq 0,
\end{cases} \]

\[ b = \left( \frac{33 m^* e^2 n_s}{8 \hbar^2 \epsilon_0 \epsilon_b} \right)^{1/3} \]

- Infinitely deep square QW

\[ V(q) = \frac{1}{A} F(q) V(q, z_0) \]

\[ F(q) = \eta^3 = \left( \frac{b}{b + q} \right)^3 \]

Form factor

- Screened scattering potential

\[ V(q, z_0) = \frac{V_{uns}(q, z_0)}{\epsilon_{2d}(q)} \]

\[ \epsilon_{2d}(q) = \epsilon(0) \left( 1 + \frac{q T F}{q} G(q) \right) \]

\[ G(q) = \frac{1}{8} \left( 2\eta^3 + 3\eta^2 + 3\eta \right) \]

Screening form factor
Handling Diffusive Transport in Low-Dimensions

Example: Remote Impurity Scattering (2DEG)

\[
V(r) = \frac{e^2}{4\pi \varepsilon} \frac{1}{\sqrt{r^2 + z^2}}
\]

Screened remote Coulomb potential

\[
V(q) = \frac{V(q, z_0)}{\epsilon_{2d}(q)} = \int_0^\infty r dr \int_0^{2\pi} d\theta \frac{e^2}{4\pi \epsilon(q) \sqrt{r^2 + z_0^2}} e^{iqr \cos \theta} = \frac{e^2}{2\epsilon_0 \epsilon(0)} \frac{e^{-q z_0}}{q + q_T F}
\]

Scattering rate (note dependence on \(k_F\))

\[
\frac{1}{\tau_{\text{rem}}(k_F)} = N_s \frac{m^*}{2\pi \hbar^2 k_F} \left( \frac{e^2}{2\epsilon_0 \epsilon(0)} \right)^2 \int_0^{2k_F} dq \frac{F(q)e^{-2q \tau_0}}{(q + q_T F G(q))^2} \frac{q^2}{\sqrt{1 - \left( \frac{q}{2k_F} \right)^2}}
\]

Averaging over distribution: No averaging necessary for degenerate 2DEGs because transport occurs by electrons at the Fermi energy!

\[-\frac{\partial f_0(E)}{\partial E} \approx \delta(E - E_F) \rightarrow \mu_{2DEG} \approx \frac{q \tau_m(k_F)}{m^*}\]
High Field Transport: Current/velocity Saturation

Hot-electron temperature: models non-equilibrium

Energy balance eqn.

Momentum balance eqn.

Steady state

Ensemble saturation velocity ~ \( (E_{\text{op}}/m^*)^{1/2} \)

However(!): Unanswered questions -
- Story not complete yet…
- Is saturation velocity independent of carrier concentrations? Not clear…
- Monte-Carlo simulations necessary for accurate high-field transport modeling.

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Outline

Part I: Review of fundamentals
1: Review of classical and quantum mechanics
2: Current flow in quantum mechanics
3: Quantum statistics, quest for equilibrium as the driver for transport

Part II: Single-particle transport
4: Ballistic transport: Quantized conductance, Ballistic MOSFETs
5: Transmission and tunneling, Tunneling FETs
6. Closed vs. open systems, the Non-Equilibrium Green’s Function approach to transport
7. Diffusive transport: Boltzmann transport equation, scattering, electron-phonon interactions
8. High-field effects, Gunn diodes and oscillators for high-frequency power

Part III: Many-particle correlated transport
9: Fock-space way of thinking transport, second quantization, conductance anomalies
10: BCS theory of superconductivity, Josephson junctions
11: Landau/Ginzburg theories of phase transitions due to broken symmetry

Part III: Geometrical and topological quantum mechanics, unification with relativity
12: Spin, transport in a magnetic field, Quantum Hall effect, Berry phase in quantum mech
13: Chern numbers, Edge/Topological states, Topological insulators and Majorana Fermions
Boltzmann Transport and beyond

$$\sigma_0 = q^2 g(E_F) D_0 = \frac{q^2 n \tau}{m} \rightarrow \sigma_0 + \Delta \sigma$$

- Boltzmann electrical conductivity
- Electronic density of states
- Diffusion coefficient
- Boltzmann/Drude result
- Weak localization quantum corrections
Some experiments BTE is unable to explain

The Aharonov-Bohm Effect

\[ G = \frac{2q^2}{h} \left[ T_0 + T_1 \cos\left( n\pi + 2\pi \frac{\Phi}{\Phi_0} \right) \right] \]

BTE methods fail to explain…
• The Aharonov Bohm effect on conductance oscillations.
• Corrections to conductivity called the weak localization.

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Weak localization corrections to conductivity

The quantum interference corrections to resistance can be written in the form

\[ \frac{\Delta R(T,H)}{R_0} = \frac{e^2}{\pi^2} \frac{R_0}{W} f(T,H). \] (1a)

Resistance goes down with increasing magnetic field

FIG. 1. Magnetoresistance data for \( L_1 \) films varying in width, \( W \), down to 0.03 ± 0.01 μm.
Path Integral approach to Quantum Mechanics

Step 1: Find the Lagrangian
\[ \mathcal{L}(x, \dot{x}) = \frac{1}{2} m \dot{x}^2 - V(x) \]

Step 2: Find the classical action along a path
\[ S_{ab} = \int_{a}^{b} dt \mathcal{L}[x, \dot{x}] \]

Step 3: Sum the quantum phases of all possible paths and get the transition amplitude
\[ \langle b|a \rangle = \sum_{\text{all paths } a \rightarrow b} A e^{i \frac{\hbar}{\hbar} S_{\text{path}}} \]

Feynman proved that the path integral approach is equivalent to the Schrödinger formulation of quantum mechanics.

Schrodinger equation for quantum mechanics
\[ i\hbar \frac{\partial |\psi\rangle}{\partial t} = \left[ \frac{\hat{p}^2}{2m} + V(r, t) \right] |\psi\rangle \]
Path integral solution to the Aharonov-Bohm problem

Lagrangian with a magnetic vector potential
\[ \mathcal{L} = \frac{1}{2}mv^2 + q\mathbf{v} \cdot \mathbf{A} - qV(\mathbf{r}) \]

‘Action’ has ‘non-magnetic’ and magnetic parts
\[ S_{ab} = S_{ab}(\mathbf{A} = 0) + q \int_a^b d\mathbf{r} \cdot \mathbf{A} \]

Obtain the path integral amplitudes for each path
\[ \langle b|1|a \rangle = \sqrt{T_1} e^{i \frac{\hbar}{\hbar} (S_{1a}^1 + S_1(\mathbf{A}))} \]
\[ \langle b|2|a \rangle = \sqrt{T_2} e^{i \frac{\hbar}{\hbar} (S_{2a}^2 + S_2(\mathbf{A}))} \]

Sum all paths to obtain the total amplitude, and then take modulus square to get the probability
\[ T = |t|^2 = |\langle b|1|a \rangle + \langle b|2|a \rangle|^2 = T_1 + T_2 + \sqrt{T_1} \sqrt{T_2} e^{i(\theta_1 - \theta_2)} e^{i \frac{\hbar}{\hbar} (S_1(\mathbf{A}) - S_2(\mathbf{A}))} + \text{c.c.} \]

The total transmission probability is the sum of the Feynman path amplitudes for the two paths connecting a and b.
**Path integral solution to the Aharonov-Bohm problem**

\[
T = |t|^2 = |\langle b|1|a\rangle + \langle b|2|a\rangle|^2 = T_1 + T_2 + \sqrt{T_1} \sqrt{T_2} e^{i(\theta_1 - \theta_2)} e^{i \frac{\pi}{\hbar} (S_1(A) - S_2(A))} + c.c.
\]

**Transmission from the path integral approach**

\[
S_1(A) - S_2(A) = q(\int_a^b dr \cdot A)_1 - q(\int_a^b dr \cdot A)_2 = q \int_a^b dr \cdot A = q \Phi
\]

**Action path integral around a loop = Magnetic Flux!**

\[
\Delta S = q \int dS \cdot B = q \int dS \cdot (\nabla \times A) = q \int dS \cdot B = q \Phi
\]

**\(\Phi_0 = \frac{\hbar}{2e}\) is the magnetic flux quantum**

\[
T = |t|^2 = T_0 + 2T_\omega \cos(\phi_0 + 2\pi \frac{\Phi}{\Phi_0})
\]

\[
G = \frac{2q^2}{\hbar} T = \frac{2q^2}{\hbar} \left[T_0 + 2T_\omega \cos(\phi_0 + 2\pi \frac{\Phi}{\Phi_0})\right]
\]

**phase \(\phi_0\) is locked to integer multiples of \(\pi\)**

\[G(\Phi) = G(-\Phi) \quad \phi_0 = n\pi\]

**Aharonov-Bohm Conductance oscillations with magnetic field**
**Schrodinger equation = Feynman path integral**

\[ i\hbar \frac{\partial}{\partial t} |i\rangle = \hat{H} |i\rangle \]

\[ |\psi(t)\rangle = \hat{U}(t) |i\rangle = e^{-\frac{i}{\hbar} \hat{H} t} |i\rangle \]

The quantum state evolves in time from its initial state.

\[ G(i, f; t) = \langle f | \psi(t) \rangle = \langle f | e^{-\frac{i}{\hbar} \hat{H} t} |i\rangle \]

The Green’s function propagator is the transition amplitude.

\[ \hat{U}(t) = e^{-\frac{i}{\hbar} \hat{H} t} \]

The time-evolution operator that acts on the initial state vector and “rotates” it into the new state in time t along a path in space and time.

\[ \hat{U}(\frac{t}{2}) \hat{U}(\frac{t}{2}) = \hat{U}(t) \]

The time evolution operator when the time is sliced into two equal parts can be decomposed into a product of two evolutions.

\[ 1 = \int dx |x\rangle \langle x| \]

Path integral with time sliced into two parts. The state vector takes all paths from \( x_i \rightarrow x \), and then all paths from \( x \rightarrow x_f \).

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Schroedinger equation = Feynman path integral

\[ \Delta t = t_n - t_{n-1} = \frac{t}{N} \]

Slice time into many infinitesimal parts

\[ x_i \rightarrow x_1 \rightarrow x_2 \rightarrow \ldots \rightarrow x_k \rightarrow x_{k+1} \rightarrow \ldots \rightarrow x_{N-1} \rightarrow x_f \]

And space into corresponding "continuous" paths

Figure 41.2: Feynman paths for path integrals.

\[
\langle x_f | e^{-\frac{i}{\hbar} \hat{H} t} | x_i \rangle = \langle x_f | e^{-\frac{i}{\hbar} \hat{H} \Delta t} \underbrace{e^{-\frac{i}{\hbar} \hat{H} \Delta t} \ldots e^{-\frac{i}{\hbar} \hat{H} \Delta t}}_{\text{N terms}} | x_i \rangle
\]

\[
\langle x_f | e^{-\frac{i}{\hbar} \hat{H} t} | x_i \rangle = \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_{N-1} \langle x_f | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x_{N-1} \rangle \ldots \langle x_2 | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x_1 \rangle \langle x_1 | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x_i \rangle
\]

\[ e^{-\frac{i}{\hbar} \hat{H} \Delta t} \approx 1 - \frac{i}{\hbar} \hat{H} \Delta t \]

"Taylor" expansion; rigorous justification in the Trotter-Lie products of Matrices

\[
\langle x_{k+1} | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x_k \rangle \approx \langle x_{k+1} | 1 - \frac{i}{\hbar} \hat{H} \Delta t | x_k \rangle
\]

\[ \hat{H} = \frac{\hat{p}^2}{2m} + V(x) \]

Hamiltonian operator acting on states gives numbers

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Schroedinger equation = Feynman path integral

\[ \Delta t = t_n - t_{n-1} = \frac{t}{N} \]

Slice time into many infinitesimal parts

\[ x_i \rightarrow x_1 \rightarrow x_2 \rightarrow \ldots \rightarrow x_k \rightarrow x_{k+1} \rightarrow \ldots \rightarrow x_{N-1} \rightarrow x_f \]

And space into corresponding “continuous” paths

Use \(1-u \sim \exp[-u]\)

**Figure 41.2:** Feynman paths for path integrals.

\[ \langle x_{k+1} | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x_k \rangle \approx \langle x_{k+1} | \left[ 1 - \frac{i}{\hbar} \hat{H} \Delta t \right] | x_k \rangle \]

\[ \hat{H} = \frac{\hat{p}^2}{2m} + V(x) \]

Time slicing

\[ \langle x_{k+1} | x_k \rangle = \delta(x_k - x_{k+1}) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ik(x_{k+1} - x_k)} \]

\[ \langle x_{k+1} | V(x) | x_k \rangle = \delta(x_k - x_{k+1}) V(x_k) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ik(x_{k+1} - x_k)} V(x_k) \]

\[ \langle x_{k+1} | \frac{\hat{p}^2}{2m} | x_k \rangle = \int_{-\infty}^{+\infty} dk \langle x_{k+1} | \frac{\hbar^2 \hat{k}^2}{2m} | k \rangle \langle k | x_k \rangle = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ik(x_{k+1} - x_k)} \frac{\hbar^2 k^2}{2m} \]

\[ \langle x_{k+1} | 1 - \frac{i}{\hbar} \hat{H} \Delta t | x_k \rangle = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ik(x_{k+1} - x_k)} \left[ 1 - \frac{i\Delta t}{\hbar} \left( V(x_k) + \frac{\hbar^2 k^2}{2m} \right) \right] \]

\[ \rightarrow \exp \left[ -\frac{i\Delta t}{\hbar} \left( V(x_k) + \frac{\hbar^2 k^2}{2m} \right) \right] \]
Feynman path integral = Schrödinger equation

\[ \langle x_{k+1} | 1 - \frac{i}{\hbar} \hat{H} \Delta t | x_k \rangle = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \cdot e^{ik(x_{k+1} - x_k)} \cdot \left[ 1 - \frac{i\Delta t}{\hbar} \left( V(x_k) + \frac{\hbar^2 k^2}{2m} \right) \right] \rightarrow \exp \left[ -\frac{i\Delta t}{\hbar} \left( V(x_k) + \frac{\hbar^2 k^2}{2m} \right) \right] \]

\[ \langle x_{k+1} | 1 - \frac{i}{\hbar} \hat{H} \Delta t | x_k \rangle \rightarrow \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \cdot \exp \left[ -\frac{i\Delta t}{\hbar} \frac{\hbar^2 k^2}{2m} + ik(x_{k+1} - x_k) - \frac{i\Delta t}{\hbar} V(x_k) \right] \]

\[ \int_{-\infty}^{+\infty} du \cdot e^{-au^2 + bu + c} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a} + c} \]  

Gaussian integral

Note the appearance of the Lagrangian!

Starting from the time-dependent Schrödinger Equation, we have arrived at the Feynman path integral.
Weak Localization in Quantum Transport

- Resistance increases at the lowest temperatures
- The increases in resistance is suppressed upon applying a magnetic field
- This sort of behavior is not possible to explain by a Boltzmann theory that tracks the probability of the electron $f(r,k,t)$ and NOT the amplitude of the electron wave!

Experimental observation of weak localization for disordered metals and doped semiconductors:

\[ \sigma_0 = q^2 g(E_F) D_0 = \frac{q^2 n \tau}{m} \rightarrow \sigma_0 + \Delta \sigma \]

- Boltzmann electrical conductivity
- Electronic density of states
- Diffusion coefficient
- Boltzmann/Drude result
- Weak localization quantum corrections

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A classical free particle moves by random scattering events and undergoes diffusive motion.

The volume spanned by classical diffusion is obtained by solving the diffusion equation.

This diffusion volume has a strong dependence on how many dimensions the particle is free to diffuse.

\[
\frac{\partial}{\partial t} P(r, t) = D \nabla^2 P(r, t)
\]

\[
D = v^2 \tau / d
\]

\[
P(r, t = 0) = \delta(r) \text{ leads to }
\]

\[
P(r, t) = \frac{1}{(4\pi Dt)^{d/2}} e^{-\frac{|r|^2}{4Dt}}
\]

\[
L = \sqrt{Dt}
\]

\[
V_{cl} \sim (Dt)^{d/2}
\]

A classical free particle moves by random scattering events and undergoes diffusive motion.

The volume spanned by classical diffusion is obtained by solving the diffusion equation.

This diffusion volume has a strong dependence on how many dimensions the particle is free to diffuse.
Quantum: Open paths interfere destructively

Path integral approach of Feynman provides the recipe for a transition of the particle from A to B. We first sum the amplitudes of each path, and then take the modulus squared for the probability. This leads to classical ‘particle’ terms, and wave-like interference terms.

\[ W_{A \to B} = | \sum_i A_i |^2 = \sum_i |A_i|^2 + \sum_{i \neq j} A_i A_j^* \]

\[ V = 0 \Rightarrow L_i = \int dt \frac{mv^2}{2} \sim p_F L_i \Rightarrow mv \sim p_F = \hbar k_F \Rightarrow A_i \sim e^{ik_F L_i} = e^{i2\pi \frac{L_i}{\lambda_F}} \]

\[ \sum_{i \neq j} A_i A_j^* = \sum_{i \neq j} e^{ik_F (L_i - L_j)} \Rightarrow \theta_{ij} = 2\pi k_F (L_i - L_j) \Rightarrow \sum_{i \neq j} A_i A_j^* = 0 \]

\[ l_{\phi} \sim v_F \tau_{\phi} \]

\[ l_{el} \sim v_F \tau_{el} \]

\[ k_F l_{el} >> 1; \text{ this is the Ioffe-Regel criterion} \]

\[ l_{\phi} >> L_i >> l_{el} \]

Condition for weak localization to occur. Obtained at low T.

Phase coherence length

Elastic mean free path

Standard open path amplitude terms interfere destructively to zero.
Closed paths interfere constructively!

\[ P(r, t) \sim \sqrt{D}t \]

- Closed loops contribute unity amplitude terms in the path integral sum. They enhance the probability of a particle to return to a starting position (say 'O'), or that of backscattering. For example, this increases the probability of finding the particle at O, decreasing the probability of transport from A to B. This means a reduction in the conductivity.

\[ W_{A\rightarrow B} = |\sum_i A_i|^2 = \sum_i |A_i|^2 + \sum_{i\neq j} A_i A_j^* \]

\[ \sum_{i\neq j} A_i A_j^* = \sum_{i\neq j} e^{ik_F(L_i-L_j)} \]

\[ e^{ik_F(\mathbf{L}_0-\mathbf{L}_0)} = 1! \]

A self-intersecting loop will interfere constructively because the time-reversed path is exactly the same length!
Enhanced backscattering due to wave-nature

\[ V_{cl} \sim (Dt)^{\frac{d}{2}} \quad dV_{int} \sim \lambda_F^{d-1}v_Fdt \]

\[ \sigma_0 = e^2g(E_F)D = e^2g(E_F)\frac{v_{F}^2\tau_{el}}{d} \]

\[ g(E_F)E_F \sim k_F^d \quad g(E_F) \sim \frac{2m}{\hbar^2}k_F^{d-2} \]

The sign of weak localization correction is negative for the existence of self-intersecting loops.

The ratio of the weak localization correction to conductivity to Drude conductivity is found geometrically.

The volume swept by the tube formed by the wave in a self-intersecting loop is proportional to the reduced conductivity.

The ratio of the back-scattered volume to the total classical diffusion volume is the conductivity correction ratio.

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Weak Localization in Quantum Transport

- The weak localization correction to the conductivity is of the ‘order’ of the quantum of conductance, and is \textbf{negative}.
- The correction is heavily dependent on the dimensionality.

\[
\frac{\delta \sigma}{\sigma_0} \sim \int_{\tau_{el}}^{\tau_{\phi}} \frac{\lambda_F^{d-1} v_F dt}{(Dt)^{d/2}}
\]

\[\delta \sigma \sim \frac{e^2}{\hbar} \times \int_{\tau_{el}}^{\tau_{\phi}} \frac{D dt}{(Dt)^{d/2}}\]

\[L_{\phi} = \sqrt{D \tau_{\phi}}\]

- For \(d = 1\), \(\delta \sigma \sim \frac{e^2}{\hbar} \times L_{\phi}\)
- For \(d = 2\), \(\delta \sigma \sim \frac{e^2}{\hbar} \times \ln\left(\frac{\tau_{\phi}}{\tau_{el}}\right)\)
- For \(d = 3\), \(\delta \sigma \sim \frac{e^2}{\hbar} \times \frac{1}{L_{\phi}}\)

\textbf{Phase diffusion length}