Quantum Conductance

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March 22, 2009
Introduction

The concept of conductance is used to explain the manner in which electrical current flows through a material. The original theory of conductance was developed in 1900 by Paul Drude. Drude’s theory did not take into account the rules of quantum mechanics which at the time were still under development. It would not be until 1925 that Pauli would introduce his exclusion principle and 1927 that Heisenberg would develop matrix mechanics and the uncertainty principle. This allowed the classical conductance theory to dominate for quite some time. Once quantum mechanics became the forerunner of physics on the atomic scale nearly every theory of classical atomic mechanic was revised including conductance.

This paper will discuss the classical theory of conductance and how it fails to provide the details necessary to link the theory and with experimental data. This theory was later replaced with the quantum theory of conductance, which solves the problems left behind by the classical theory. This theory will be discussed along with the concepts that are required to understand this explanation.

Particles and Forces

The quantum theory of conductance was a revolution in thinking as it departed from the classical mentality that atoms were rigid balls. In understanding all that is encompassed with this theory, let us start with an introduction to the elementary particles, the force carriers and the fundamental forces.

A description of the fundamental particles will help to understand a few concepts in quantum conduction, so we will start with table one.
Matter is composed of fermions. The table above shows the 12 types of fermions that exist. Each of the fermions also have an anti matter counterpart. The fermions break down into leptons and quarks. The leptons do not combine to form other particles but the quarks form hadrons. There are two types of hadrons, the baryons and the mesons. Mesons are formed by quark anti-quark pairs where baryons are formed by three quark combinations. Protons and neutrons are from the baryon family.

The force carriers are the gluon, photon and the bosons. These particles, along with the graviton (theoretical force carrier of gravitation) and the Higg’s boson (theoretical particle said to give particles their mass), make up the standard model of physics. We need not go into depth with these particles, but there are a few important points.

Fermions are particles with half integer spins and the force carriers have full integer spins. This is very important because the particles with half integer spin are governed by the Pauli exclusion principle while the full integer particles are not.

The force carriers are responsible for propagating the four forces of the universe. These forces are shown below in table two.

Table 1: Elementary Particles and Force Carriers

<table>
<thead>
<tr>
<th>Quarks</th>
<th>Leptons</th>
<th>Bosons (Forces)</th>
</tr>
</thead>
<tbody>
<tr>
<td>u up</td>
<td>e electron</td>
<td>W weak force</td>
</tr>
<tr>
<td>d down</td>
<td>μ muon</td>
<td>Z weak force</td>
</tr>
<tr>
<td>c charm</td>
<td>μ muon</td>
<td>Z weak force</td>
</tr>
<tr>
<td>t top</td>
<td>τ tau</td>
<td>Z weak force</td>
</tr>
<tr>
<td>y photon</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Three Generations of Matter (Fermions)

- Mass: 2.4 MeV, 4.8 MeV, <77 eV
- Charge: \( \frac{2}{3}, \frac{1}{2}, 0 \)
- Spin: \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)
- Name: u, d, c, t, y

<table>
<thead>
<tr>
<th>Mass</th>
<th>Charge</th>
<th>Spin</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.4 MeV</td>
<td>( \frac{2}{3} )</td>
<td>( \frac{1}{2} )</td>
<td>u up</td>
</tr>
<tr>
<td>4.8 MeV</td>
<td>( \frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>d down</td>
</tr>
<tr>
<td>2.7 GeV</td>
<td>( \frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>c charm</td>
</tr>
<tr>
<td>17.2 GeV</td>
<td>( \frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>t top</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>y photon</td>
</tr>
</tbody>
</table>

### Table 2: Forces of the Universe

- **Electromagnetic Force**: Carried by the photon. 
- **Weak Nuclear Force**: Carried by the W and Z bosons. 
- **Strong Nuclear Force**: Carried by the gluons. 
- **Gravitational Force**: Carried by the graviton (theoretical particle)

<table>
<thead>
<tr>
<th>Force</th>
<th>Carrier</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electromagnetic</td>
<td>Photon</td>
</tr>
<tr>
<td>Weak Nuclear</td>
<td>W, Z</td>
</tr>
<tr>
<td>Strong Nuclear</td>
<td>Gluons</td>
</tr>
<tr>
<td>Gravitational</td>
<td>Graviton</td>
</tr>
</tbody>
</table>

These forces make up the standard model of physics.
<table>
<thead>
<tr>
<th>Interaction</th>
<th>Current Theory</th>
<th>Mediators</th>
<th>Relative Strength</th>
<th>Range(m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong</td>
<td>Quantum Chromodynamics</td>
<td>Gluons</td>
<td>$10^{38} / 10$</td>
<td>$10^{-15}$</td>
</tr>
<tr>
<td>Electromagnetic</td>
<td>Quantum Electrodynamics</td>
<td>Photons</td>
<td>$10^{36} / 10$</td>
<td>Infinite</td>
</tr>
<tr>
<td>Weak</td>
<td>Electroweak Theory</td>
<td>W and Z Bosons</td>
<td>$10^{25} / 10$</td>
<td>$10^{-18}$</td>
</tr>
<tr>
<td>Gravitation</td>
<td>General Relativity</td>
<td>Gravitons (Theoretical)</td>
<td>1</td>
<td>Infinite</td>
</tr>
</tbody>
</table>

Table 2: Fundamental Forces

When discussing conduction we must focus on the electromagnetic force which is propagated by the photon. The quest to unify these forces into one complete theory is known as grand unification.

The Heisenberg Uncertainty Principle

In 1927 Werner Heisenberg postulated the concept that the measurements of energy, time, location and momentum could only be made to a finite accuracy. He followed by explaining that the more accurate the measurement of location of a particle, the less accurate the measurement of momentum would be and vice versa. This same relationship exists between time and energy. This theory became known as the uncertainty principle. The mathematical relationship can be seen below.

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$  \hspace{1cm} (eq. 1)

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$  \hspace{1cm} (eq. 2)

Where $\hbar$ is defined as $\frac{\hbar}{2}$ and $\hbar$ is Planck’s constant and equals $6.626 \times 10^{-34}$.

Now let us take a look at a proven example that will prove the validity of these statements. Recall our discussion of the elementary particles and take note of the properties listed in table one. Here we need to be familiar with the up and down quarks as well as the W’ boson, the carrier of the weak nuclear force.

Our example is to explore beta decay. This process is common in radioactive decay. In such a case, a high energy electron is emitted when a radioactive atom splits into two or more atoms of smaller mass. When the products of such a process are examined, it is found that there is one less neutron and one more electron and proton that had existed in the original radioactive
atom. This indicates that a neutron has decayed into a proton and an electron. This is quite common; in fact, a neutron that is not bound in the nucleus of an atom will decay into a proton and electron with a half life of 14 minutes.

We again revisit our discussion of particle physics and recall that that protons and neutrons are baryons and are composed of three quarks. Quarks have a slight similarity with electrons in that they have an electromagnetic charge. Table one shows their charge. Unlike the electron, the quark is also subject to the strong nuclear force. A large majority of the mass of the proton and neutron is actually bound strong force energy. As a particle governed by the strong force, it must have strong force charge. Unlike the electromagnetic force which has two charges (positive and negative) the strong force has three charges called color charges, which are red blue and green. Actual color has nothing to do with these names; they are used just to differentiate them. Like the electromagnetic force, like charges repel and opposites attract. Because baryons have three quarks, the only way for the particle to be stable is to have one quark of each color which in turn makes a “white” or colorless baryon. Figure one shows the proton and neutron.

Proton
\[
 \text{Mass} = 938 \text{MeV}/c^2 \\
\text{Mass of quarks} = 9.6 \text{MeV}/c^2
\]

Neutron
\[
 \text{Mass} = 940 \text{MeV}/c^2 \\
\text{Mass of quarks} = 12 \text{MeV}/c^2
\]

Figure 1: Proton and Neutron Composite

It is easy to see that for the neutron to decay into a proton one of the down quarks must decay into an up quark. The difference in energy of the two particles is released is converted into an electron and a neutrino. There are a few steps to this decay process that we will now discuss. Figure two shows the full process.
Figure 2: Beta Decay

As the figure shows, during the decay process the $W^-$ boson is created. Its mass is much higher than that of the neutron. This violates the universal law of conservation of energy. However, Heisenberg tells us that this can occur if the time frame of the energy discrepancy is on an order defined by the uncertainty principle. Equations three through six show the time frame in question.

$$\frac{\hbar}{2} = 3.29 \cdot 10^{-16} \text{ eV} \cdot \text{s}$$  \hspace{1cm} (eq. 3)

$$\Delta E \cdot \Delta t \geq 3.29 \cdot 10^{-16} \text{ eV} \cdot \text{s}$$  \hspace{1cm} (eq. 4)

$$80.4 \cdot 10^9 \text{ eV}/c^2 \cdot \Delta t \geq 3.29 \cdot 10^{-16} \text{ eV} \cdot \text{s}$$  \hspace{1cm} (eq. 5)

$$\Delta E = 4.10 \cdot 10^{-27} \text{ s}$$  \hspace{1cm} (eq. 6)

This time frame only allows the boson to travel about $10^{-18}$ meters. That is only about a thousandth of the diameter of a proton. This analysis not only shows how beta decay occurs but also validates the uncertainty principle. It has also been confirmed experimentally.

The Pauli Exclusion Principle

As scientists began to explore more in depth areas of the emerging quantum mechanics theories several phenomena raised questions about the fundamental laws of classical physics. The discrete nature of energy levels was one of these phenomena. This led Wolfgang Pauli to develop his exclusion principle in 1925.

As discussed previously, this principle only applies to fermions (particles with half integer spin). The principle states that no two identical fermions can occupy the same quantum state at the same time within the same system. The quantum state is described by four values. The first
value “n” refers to the energy shell and the value of ℓ denotes the sub-shell. The angular momentum is classified by \( m_\ell \) and \( m_s \) denotes the spin.

This principle requires that only a few electrons will be in the energy level that contributes to conduction. This principle plays an important part in the quantum theory of conductance. In a conducting material of identical atoms, it is the electrons in the highest energy level that contribute to conduction. The exclusion principle says that these electrons cannot have the same quantum state. Because of this principle, the electrons will take on slightly different energies. When a large number of atoms exist in the quantum system, the difference in energy of the electrons falls into the range of the uncertainty principle. This means that the electrons’ exact energy (while slightly different) cannot be experimentally measured. Figure three shows the difference between conducting, semi-conducting and insulating band gaps.

![Figure 3: Band Gaps](image)

This figure shows the bands created by the need for the energy level splitting. If this figure represented a single atom, the bands would shrink to a single line. However, because there are many atoms in a conductor, the exclusion principle dictates the existence of these bands.

**Classical Conduction**

The classical theory of conduction was developed in 1900 by Paul Drude. This theory states that a conductor must have free electrons to contribute to the flow of current. These free electrons move though the conductors like a gas. They have a mean velocity of zero because of the random direction of the movement, while the mean speed is quite high. When an electric field is placed on the conductor, the cloud of electrons will move from high potential to low potential. Along the path of travel, the electrons move and collide with lattice ions and then move again. This collision and acceleration pattern is what limits the flow of current and
creates conductor resistance. The movement of the electrons is referred to as the drift velocity.

In the classical theory, several equations are developed that describe the resistivity and conductance. These equations are useful in developing Ohm’s law; however, they make no mention of the linear relationship with temperature, and the conductance and resistivity are nearly an order of magnitude off from the experimentally obtained values. It was Louis de Broglie in 1924 that showed that matter acts like a wave as well as like a particle. This concept was not taken into account in the classical theory.

Quantum Conductance

After the theories of quantum mechanics were developed, a new interpretation of conductance was developed. This theory takes into account the principles we have discussed to this point. We will begin by deriving the equation for conductance.

$$G = \frac{I}{\Delta V}$$  \hspace{1cm} (eq. 7)

Equation seven shows the definition of conductance. Here $I$ is current and $V$ is voltage. Equations eight and nine show the definition of voltage and current.

$$I = \frac{nq}{\Delta t}$$  \hspace{1cm} (eq. 8)

$$\Delta V = \frac{\Delta U}{q}$$  \hspace{1cm} (eq. 9)

Here $n$ represents the number of electrons, $q$ is the charge of an electron ($1.602 \cdot 10^{-19}$C), $t$ is time and $U$ is the electrostatic charge. By substituting equation eight and nine into equation seven we get equation 10.

$$G = \frac{nq}{\Delta t \frac{\Delta U}{q}}$$  \hspace{1cm} (eq. 10)

This simplifies to:
Because \( \Delta U \) is simply a measure of energy we can easily replace the denominator of equation 11 with the time energy form of the uncertainty principle to obtain equation 12.

\[
G = \frac{nq^2}{\Delta U \Delta t}
\]  
(eq. 11)

Because equation one is an inequality we must change equation 11 to an inequality when performing the substitution.

\[
G \geq \frac{nq^2}{\hbar} \frac{1}{2}
\]  
(eq. 12)

The simplified value is shown in equation 13 and all the variables are constant except \( n \). To determine this value we return to the exclusion principle. It is only the electrons in the highest energy level that can be promoted to the conduction band. In terms of energy it is the first three quantum numbers that denote electron energy. The fourth number is the quantum spin and does not quantify energy. This means only two electrons can have the same energy (the same first three quantum numbers), one with spin up and one spin down.

When promoted to the conduction band, the wave like properties of the electron would allow them to pass though the conduction lattice with no resistance provided the lattice was free from defects and the wavelength of the electrons was greater than the lattice spacing. These electrons are in a position to jump to the next energy level and begin conduction. They gain the energy though a kinetic energy transfer. At all non-zero temperatures, the lattice ions will move with some kinetic energy denoted by \( kT \) where \( k \) is the Boltzmann constant (1.38-10⁻²³ m²kg/s²k) and \( T \) is the temperature in Kelvin. When an electron bumps into a lattice ion, this is the maximum energy that can be transferred and it follows that only the electrons that have an energy within \( kT \) of the conduction band energy can be promoted. In semi-conductors, these electrons need a little extra help to be promoted and for the insulators this promotion requires a catastrophic amount of energy enough energy that that structure of the insulator would be altered by such an input of energy.
This promotion in energy level alters the wave function of the electron and in turn alters the way the electrons behave. This new conduction band electron will propagate though the conductor from high to low potential. Even if the conductor is free from structural flaws and impurities, it is still not free from imperfections as the movement of the ions in the lattice acts to scatter the electrons. It is these scattering events that limit the flow of electricity in a conductor. Because only a few electrons are within kT of the Fermi level, there are only a few electrons that can be promoted. When looking at the minimum degree of conduction, we will look only at the electrons of the highest level and assume that they are the only ones that can be promoted to conduction. The highest energy level will hold two electrons giving us a value for \( n \) in equation 13. While it is possible that more electrons will be promoted to conduction we are after the minimum amount of conduction which would require the smallest number of electrons.

Now we can solve equation 13 for \( G \). Equation 14 shows the relationship between conductance and resistance.

\[
R = \frac{1}{G}
\]

(eq. 14)

Substituting equation 14 in 13 we have:

\[
R \geq \frac{\hbar}{2nq^2}
\]

(eq. 15)

This yields the final result of the resistance of a conductor that is one atom thick where only the highest energy electrons can contribute to conduction.

\[
R \geq 1027.3 \, \Omega
\]

(eq. 16)

This value can be modified and will at time be seen written in a slightly different form. If equation one and two were set greater than \( h \) instead of \( h/2 \) than we have:

\[
R \geq \frac{\hbar}{nq^2}
\]

(eq. 17)
This leads to:

\[ R \geq 12.9 \, \text{k}\Omega \] (eq. 18)

Generally speaking the equation one and two are in the accepted form. This form was not developed by Heisenberg but was instead shown to be true after the original uncertainty principle postulated. It is included here for the sake of completeness.

**Superconductors**

In the previous section, we showed that the resistance between two atoms has a finite non-zero value. However, superconductors have shown a zero resistance and an unimpeded conductance. We made the assumption that only two electrons could be promoted to the conduction band. If we, however, modify this assumption in order for equation 15 to equal zero, \( n \) would go to infinity which is not possible.

This creates an interesting question. Why does a superconductor have a zero resistance and hence a zero resistivity? For that answer we will take a look at BCS theory. BCS theory was developed by John Bardeen, Leon Cooper and John Schrieffer in 1948. In essence, the theory states that superconductivity is a macroscopic effect of the Bose condensation of a pair of electron. These electrons will take on the properties of a boson. Recall the bosons on table one. They are full integer spin particles and are not considered fermions. This property excludes them from the restriction set down by the Pauli Exclusion Principle. We assumed that electrons could not have the same quantum state which dictated the need for slight energy changes for electrons to move from state to state. However, bosons do not have this restriction and would be able to move about freely without the need of an external potential to push them along.

**Effects of Quantum Conductance**

The resistance created by quantum conductance can cause a number of undesired effects with respect to nano-technology. These effects can be demonstrated with an example. Consider a microprocessor designer who wishes to use molecular transistors in a new design. The design, in theory, calls for the flow of current across a carbon-carbon bond. Let us take a look at some numbers that will bring this example to light.

The design parameters call for this transistor to operate at 3 GHz. Current flow is measured in amperes and one ampere equates to \( 6.242 \times 10^{18} \) electrons passing a cross sectional area per second. Now consider equations 19 through 21.
\[ V = \frac{J}{C} \quad \text{(eq. 19)} \]
\[ I = \frac{C}{S} \quad \text{(eq. 20)} \]
\[ V = IR \quad \text{(eq. 21)} \]

Equation 19 shows the joules per coulomb relationship of voltage while equation 20 shows the coulomb per second relationship of current. Equation 21 is the familiar Ohm’s Law.

If this hypothetical processor is to work at 3 GHz it would need at least one electron to flow for each transition. This means at least \(3 \times 10^9\) electrons must flow per second at maximum. Equation 22 shows how much current is flowing.

\[
\frac{3 \times 10^9 \text{ e}^-}{6.242 \times 10^{18} \text{ e}^-/\text{A}} = 4.8062 \times 10^{-10} \text{ A}
\quad \text{(eq. 22)}
\]

Moving along we will use this current and the resistance obtained in equation 16 to solve Ohm’s Law.

\[
1027.3 \Omega \cdot 4.8062 \times 10^{-10} \text{ A} = 4.9374 \times 10^{-7} \text{ V}
\quad \text{(eq. 23)}
\]

Now we will calculate the total charge by multiplying the charge of an electron by the total number of electrons.

\[
1.602 \times 10^{-19} \text{ C/e}^- \cdot 3 \times 10^9 \text{ e}^- \quad \text{(eq. 24)}
\]

Using the solution from equation 23 and 24 we will now solve equation 19 for the energy.

\[
4.9374 \times 10^{-7} \text{ V} \cdot 4.806 \times 10^{-10} \text{ C} = 2.3729 \times 10^{-16} \text{ J}
\quad \text{(eq. 25)}
\]

Now let us take a look at the carbon-carbon bond. This bond has an energy of more than 600 kJ/mol. If we divide this number by Avogadro’s number we will obtain the energy per bond.
\[
\frac{606.68 \text{ kJ/mol}}{6.022 \cdot 10^{23} \text{ bonds/mol}} = 1.0074 \cdot 10^{-18} \text{ J/bond}
\]

(eq. 26)

A comparison of the results from equations 25 and 26 we see that at 3 GHz the current required is two orders of magnitude high that the bond would allow before breaking.

This problem could be overcome with a different molecule but its effect is evident in the current state of nano technology. The *International Technology Roadmap for Semi-conductors* shows that single electron transistors and molecular transistors have a theoretical maximum circuit speed of one gigahertz. This is much slower that the current state of the art. Their size, however, allows them to be packed in tightly enough to create multiple core systems that are superior than what is currently available.

The effects of quantum conductance show a clear obstacle in nano technology and must be overcome by new thinking and new designs if the current state of the art is to continue expanding in accordance with Moore’s Law.