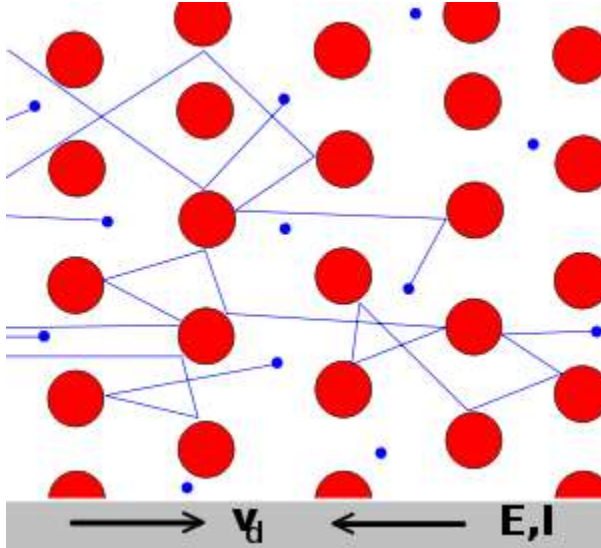


# Drude theory of conduction



Drude Model electrons (shown here in blue) constantly bounce between heavier, stationary crystal ions (shown in red).

The **Drude theory(model)** of electrical conduction was proposed in 1900<sup>[1][2]</sup> by Paul Drude to explain the transport properties of electrons in materials (especially metals). The model, which is an application of kinetic theory, assumes that the microscopic behavior of electrons in a solid may be treated classically and looks much like a pinball machine, with a sea of constantly jittering electrons bouncing and re-bouncing off heavier, relatively immobile positive ions.

The two most significant results of the Drude model are an electronic equation of motion,

$$\frac{d}{dt}\mathbf{p}(t) = q\mathbf{E} - \frac{\mathbf{p}(t)}{\tau},$$

and a linear relationship between current density  $\mathbf{J}$  and electric field  $\mathbf{E}$ ,

$$\mathbf{J} = \left( \frac{nq^2\tau}{m} \right) \mathbf{E}.$$

Here  $t$  is the time and  $\mathbf{p}$ ,  $q$ ,  $n$  and  $m$ , and  $\tau$  are respectively an electron's momentum, charge, number density, mass, and mean free time between ionic collisions. The latter expression is particularly important because it explains in semi-quantitative terms why Ohm's Law, one of the most ubiquitous relationships in all of electromagnetism, should be true.

The model was extended in 1905 by Hendrik Antoon Lorentz (and hence is also known as the Drude–Lorentz model) and was supplemented with the results of quantum theory in 1933 by Arnold Sommerfeld and Hans Bethe.

## Assumptions

The Drude model considers the metal to be formed of a mass of positively-charged ions from which a number of "free electrons" were detached. These may be thought to have become delocalized when the valence levels of the atom came in contact with the potential of the other atoms.

Notwithstanding the origin of such free electrons from the contact of different potentials, the Drude model neglects any long-range interaction between the electron and the ions and assumes that the electrons do not interfere with each other. The only possible interaction is the instantaneous collision between a free electron and an ion, which happens with a fixed probability per unit time.

The Drude model is a purely classical model, and treats both electrons and ions as solid spheres.

## Explanations

### DC field

The simplest analysis of the Drude model assumes that electric field  $\mathbf{E}$  is both uniform and constant, and that the thermal velocity of electrons is sufficiently high such that they accumulate only an infinitesimal amount of momentum  $d\mathbf{p}$  between collisions, which occur on average every  $\tau$  seconds.

Then an electron isolated at time  $t$  will on average have been traveling for time  $\tau$  since its last collision, and consequently will have accumulated momentum

$$d\langle\mathbf{p}\rangle = q\mathbf{E}\tau.$$

During its last collision, this electron will have been just as likely to have bounced forward as backward, so all prior contributions to the electron's momentum may be ignored, resulting in the expression

$$\langle\mathbf{p}\rangle = q\mathbf{E}\tau.$$

Substituting the relations

$$\begin{aligned}\langle\mathbf{p}\rangle &= m\langle\mathbf{v}\rangle, \\ \mathbf{J} &= nq\langle\mathbf{v}\rangle,\end{aligned}$$

results in the formulation of Ohm's Law ( $v=ir$ ) mentioned above:

$$\mathbf{J} = \left( \frac{nq^2\tau}{m} \right) \mathbf{E}.$$

### Time-varying analysis

The dynamics may also be described by introducing an effective drag force. At time  $t = t_0 + dt$  the average electron's momentum will be

$$\langle \mathbf{p}(t_0 + dt) \rangle = \left( 1 - \frac{dt}{\tau} \right) \langle \mathbf{p}(t_0) \rangle + q\mathbf{E}dt,$$

because, on average,  $(1 - dt/\tau)$  electrons will not have experienced another collision, and the ones that have will contribute to the total momentum to only a negligible order.

With a bit of algebra, this results in the differential equation

$$\frac{d}{dt} \langle \mathbf{p}(t) \rangle = q\mathbf{E} - \frac{\langle \mathbf{p}(t) \rangle}{\tau},$$

where  $\langle \mathbf{p} \rangle$  denotes average momentum and  $q$  the charge of the electrons. This, which is an inhomogeneous differential equation, may be solved to obtain the general solution of

$$\langle \mathbf{p}(t) \rangle = q\tau\mathbf{E} + \mathbf{C}e^{-t/\tau}$$

for  $\mathbf{p}(t)$ . The steady state solution ( $\frac{d}{dt} \langle \mathbf{p} \rangle = 0$ ) is then

$$\langle \mathbf{p} \rangle = q\tau\mathbf{E},$$

As above, average momentum may be related to average velocity and this in turn may be related to current density,

$$\begin{aligned} \langle \mathbf{p} \rangle &= m\langle \mathbf{v} \rangle, \\ \mathbf{J} &= nq\langle \mathbf{v} \rangle, \end{aligned}$$

and the material can be shown to satisfy Ohm's Law with a DC-conductivity  $\sigma_0$ :

$$\mathbf{J} = \left( \frac{nq^2\tau}{m} \right) \mathbf{E}.$$

The Drude model can also predict the current as a response to a time-dependent electric field with an angular frequency  $\omega$ , in which case

$$\sigma(\omega) = \frac{\sigma_0}{1 + i\omega\tau}.$$

Here it is assumed that

$$\begin{aligned} E(t) &= \Re(E_0 e^{i\omega t}); \\ J(t) &= \Re(\sigma(\omega) E_0 e^{i\omega t}). \end{aligned}$$

In other conventions,  $i$  is replaced by  $-i$  in all equations. The imaginary part indicates that the current lags behind the electrical field, which happens because the electrons need roughly a time  $\tau$  to accelerate in response to a change in the electrical field. Here the Drude model is applied to electrons; it can be applied both to electrons and holes; i.e., positive charge carriers in semiconductors. The curves for  $\sigma(\omega)$  are shown in the graph.

## Accuracy of the model

This simple classical Drude model provides a very good explanation of DC and AC conductivity in metals, the Hall effect, and thermal conductivity (due to electrons) in metals near room temperature. The model also explains the Wiedemann-Franz law of 1853. However, it greatly overestimates the electronic heat capacities of metals. In reality, metals and insulators have roughly the same heat capacity at room temperature. Although the model can be applied to positive (hole) charge carriers, as demonstrated by the Hall effect, it does not predict their existence.

One note of trivia surrounding the theory is that in his original paper Drude made a conceptual error, estimating electrical conductivity to in fact be only half of what it classically should have been.

<sup>2nd</sup> topic

### The Fermi level

It is a hypothetical level of potential energy for an electron inside a crystalline solid. Occupying such a level would give an electron (in the fields of all its neighboring nuclei) a potential energy  $\epsilon$  equal to its chemical potential  $\mu$  (average diffusion energy per electron) as they both appear in the Fermi-Dirac distribution function,

$$F_e(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/(kT)} + 1}$$

which calculates the probability that an electron with energy  $\epsilon$  occupies a particular single-particle state (density of states) within such a solid.  $T$  is the absolute temperature and  $k$  is

Boltzmann's constant. When  $\epsilon = \mu$  the exponential equals 1, and the value of  $F_e(\epsilon)$  describes the Fermi level as a state with 50% chance of being occupied by an electron for the given temperature of the solid.

Suppose we want to accommodate  $N$  electrons on the line. This can be done with the help of Pauli Exclusion Principle. In a solid the quantum nos. of an electron in a conduction electron state are  $n$  and  $m_s$ .

Every energy level with a quantum no.  $n$  can accommodate 2 electrons, one with spin up and other with spin down. eg. There are 8 electrons, then in ground state of the system the level with  $n = 1, 2, 3, 4$  are filled while higher levels ( $n > 4$ ) are empty. Suppose we start filling the levels from the bottom ( $n=1$ ) and continue filling the higher levels with  $e^-$  until all  $N$  electrons are accommodated. Let  $n_f$  denote top most filled energy level. Assuming to be even we have

$$2n_f = N$$

Which determine value of  $n$  for uppermost filled level.

‘At absolute zero all the levels below a certain level will be filled with electrons and all the level above it will be empty. The level which divides the filled and vacant levels is called Fermi level at absolute zero ‘

‘ the energy of the top most filled level at absolute zero is called Fermi energy ‘

### **Fermi level" in semiconductor physics**

In semiconductor physics it is conventional to work mainly with unreferenced energy symbols. This is possible because the relevant formulas of semiconductor physics mostly contain differences in energy levels, for example  $(E_C - E_F)$ . Thus, for developing the basic theory of semiconductors there is little merit in introducing an absolute energy reference zero. This can be qualitatively understood as asserting the importance of the encountered potential difference instead of the absolute potential difference.

### **The Fermi Dirac distribution function**

The Fermi-Dirac distribution  $f(E)$  gives the probability that a single-particle state of energy  $E$  would be occupied by an electron (at thermodynamic equilibrium): Alternatively, it also gives the average number of electrons that will occupy that state due to the restriction imposed by the Pauli exclusion principle.

$$f(E) = \frac{1}{1 + \exp\left[\frac{E - \mu}{k_B T}\right]} = \frac{1}{1 + \exp\left[\frac{\epsilon}{k_B T}\right]},$$

where:

- $\mu$  is the parameter called the chemical potential (which, in general, is a function of  $T$ );
- $\epsilon \equiv E - \mu$  is the electron energy measured relative to the chemical potential;
- $k_B$  is Boltzmann's constant;
- $T$  is the temperature.

In particular,  $f(\mu) = 0.5$ .

## Fermi–Dirac distribution

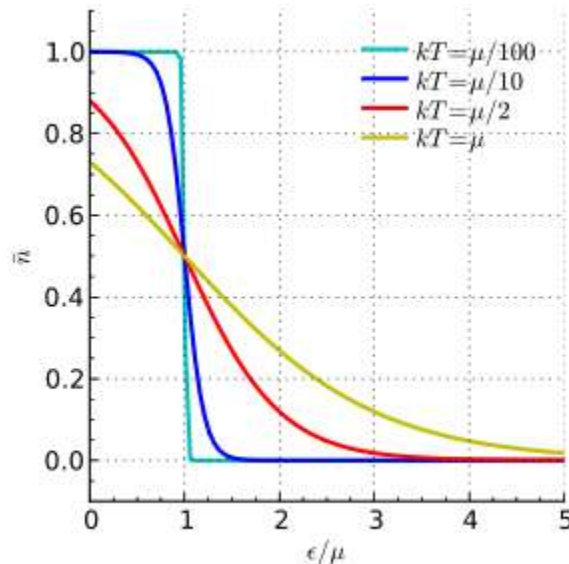
For a system of identical fermions, the average number of fermions in a single-particle state  $i$ , is given by the Fermi–Dirac (F–D) distribution,

$$\bar{n}_i = \frac{1}{e^{(\epsilon_i - \mu)/kT} + 1}$$

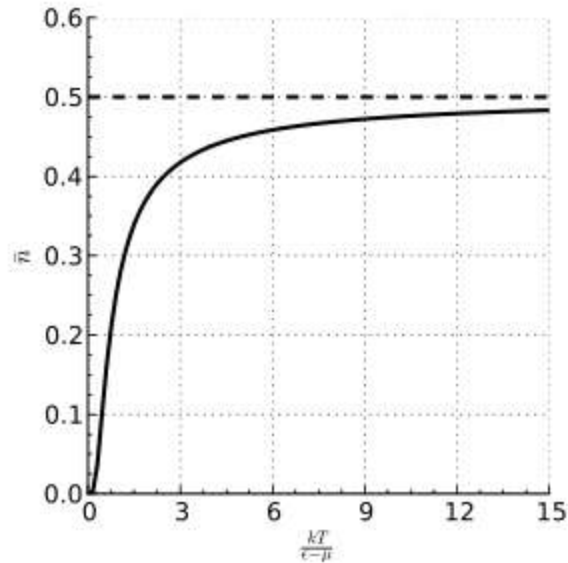
where  $k$  is Boltzmann's constant,  $T$  is the absolute temperature,  $\epsilon_i$  is the energy of the single-particle state  $i$ , and  $\mu$  is the chemical potential. At  $T = 0$  K, the chemical potential is equal to the Fermi energy. For the case of electrons in a semiconductor,  $\mu$  is also called the Fermi level.

The F–D distribution is only valid if the number of fermions in the system is large enough so that adding one more fermion to the system has negligible effect on  $\mu$ . Since the F–D distribution was derived using the Pauli exclusion principle, which allows at most one electron to occupy each possible state, a result is that  $0 < \bar{n}_i < 1$ .

- Fermi–Dirac distribution



**Energy dependence.** More gradual at higher  $T$ .  $\bar{n} = 0.5$  when  $\epsilon = \mu$ . Not shown is that  $\mu$  decreases for higher  $T$ .



• **Temperature dependence for  $\epsilon > \mu$ .**

History:

Before the introduction of Fermi–Dirac statistics in 1926, understanding some aspects of electron behavior was difficult due to seemingly contradictory phenomena. For example, the electronic heat capacity of a metal at room temperature seemed to come from 100 times fewer electrons than were in the electric current. It was also difficult to understand why the emission currents, generated by applying high electric fields to metals at room temperature, were almost independent of temperature.

The difficulty encountered by the electronic theory of metals at that time was due to considering that electrons were (according to classical statistics theory) all equivalent. In other words it was believed that each electron contributed to the specific heat an amount on the order of the Boltzmann constant  $k$ . This statistical problem remained unsolved until the discovery of F–D statistics.

F–D statistics was first published in 1926 by Enrico Fermi and Paul Dirac. According to an account, Pascual Jordan developed in 1925 the same statistics which he called *Pauli statistics*, but it was not published in a timely manner. Whereas according to Dirac, it was first studied by Fermi, and Dirac called it Fermi statistics and the corresponding particles fermions.

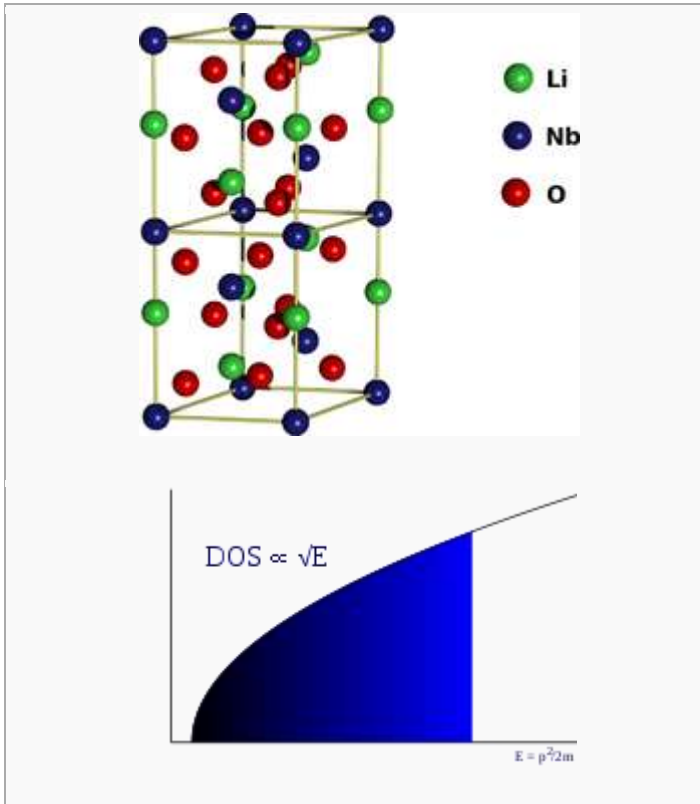
F–D statistics was applied in 1926 by Fowler to describe the collapse of a star to a white dwarf. In 1927 Sommerfeld applied it to electrons in metals and in 1928 Fowler and Nordheim applied it to field electron emission from metals. Fermi–Dirac statistics continues to be an important part of physics

3<sup>rd</sup> topic

## Density of states

‘it is defined as number of electronic states (or orbitals) per unit energy range , and is denoted by  $D(E)$

$$\text{As we know } E_n = \frac{h^2}{2m} \left(\frac{n\pi}{L}\right)^2$$



$E = \text{K.E.}$

In three dimensions, the density of states of a gas of fermions is proportional to the square root of the kinetic energy of the particles.

In solid-state and condensed matter physics, the **density of states (DOS)** of a system describes the number of states per interval of energy at each energy level that are available to be occupied by electrons. Unlike isolated systems, like atoms or molecules in gas phase, the density



distributions are not discrete like a spectral density but continuous. A high DOS at a specific energy level means that there are many states available for occupation. A DOS of zero means that no states can be occupied at that energy level. In general a DOS is an average over the space and time domains occupied by the system. Local variations, most often due to distortions of the original system, are often called **local density of states (LDOS)**. If the DOS of an undisturbed system is zero, the LDOS can locally be non-zero due to the presence of a local potential.

For electrons at the conduction band edge, very few states are available for the electron to occupy. As the electron increases in energy, the electron density of states increases and more states become available for occupation. However, because there are no states available for electrons to occupy within the bandgap, electrons at the conduction band edge must lose at least  $E_g$  of energy in order to transition to another available mode. The density of states can be calculated for electron, photon, or phonon in QM systems. The DOS is usually represented by one of the symbols  $g$ ,  $\rho$ ,  $D$ ,  $n$ , or  $N$ , and can be given as a function of either energy or wave vector  $k$ .

## Density of energy states

To finish the calculation for DOS find the number of states per unit sample volume at an energy  $E$  inside an interval  $[E, E + dE]$ . The general form of DOS of a system is given as

$$D_n(E) = \frac{d\Omega_n(E)}{dE}$$

The scheme sketched so far **only** applies to **continuously rising** and **spherically symmetric** dispersion relations. In general the dispersion relation  $E(k)$  is not spherically symmetric and in many cases it isn't continuously rising either. To express  $D$  as a function of  $E$  the inverse of the dispersion relation  $E(k)$  has to be substituted into the expression of  $\Omega_n(k)$  as a function of  $k$  to get the expression of  $\Omega_n(E)$  as a function of the energy. If the dispersion relation is not spherically symmetric or continuously rising and can't be inverted easily then in most cases the DOS has to be calculated numerically. More detailed derivations are available.

## . Applications

The density of states appears in many areas of physics, and helps to explain a number of quantum mechanical phenomena.

### Quantization

Calculating the density of states for small structures shows that the distribution of electrons changes as dimensionality is reduced. For quantum wires, the DOS for certain energies actually becomes higher than the DOS for bulk semiconductors, and for quantum dots the electrons become quantized to certain energies.

## Photonic crystals

The photon density of states can be manipulated by using periodic structures with length scales on the order of the wavelength of light. Some structures can completely inhibit the propagation of light of certain colors (energies), creating a photonic bandgap: the DOS is zero for those photon energies. Other structures can inhibit the propagation of light only in certain directions to create mirrors, waveguides, and cavities. Such periodic structures are known as [photonic crystals](#).

## Calculation of the density of states

Interesting systems are in general complex, for instance compounds, biomolecules, polymers, etc. Because of the complexity of these systems the analytical calculation of the density of states is in most of the cases impossible. Computer simulations offer a set of algorithms to evaluate the density of states with a high accuracy. One of these algorithms is called the Wang and Landau algorithm.

Within the Wang and Landau scheme any previous knowledge of the density of states is required. One proceed as follows: the cost function (for example the energy) of the system is discretized. Each time the bin  $i$  is reached one update a histogram for the density of, states  $g(i)$  ,by,

$$g(i) \rightarrow g(i) + f,$$

where  $f$  is called modification factor. As soon as each bin in the histogram is visited a certain number of times (10-15), the modification factor is reduced by some criterion, for instance,

$$f_{n+1} \rightarrow (1/2)f_n$$

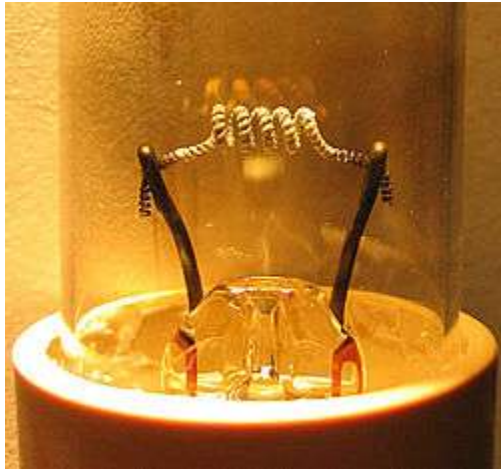
where  $n$  denotes the  $n$ -th update step. The simulation finishes when the modification factor is less than a certain threshold, for instance  $f_n < 10^{-8}$ .

The Wang and Landau algorithm has some advantages over other common algorithms such as multicanonical simulations and Parallel tempering, for instance, the density of states is obtained as the main product of the simulation. Additionally, Wang and Landau simulations are completely independent of the temperature. This feature allows to compute the density of states of systems with very rough energy landscape such as proteins.

4<sup>th</sup> topic

## Thermionic emission

**The phenomenon of emission of electrons from the surface of the metal, when it is heated, is called thermionic emission .**



Close up of the filament on a low pressure mercury gas discharge lamp showing white thermionic emission mix coating on the central portion of the coil. Typically made of a mixture of barium, strontium and calcium oxides, the coating is sputtered away through normal use, often eventually resulting in lamp failure.

**Thermionic emission** is the heat-induced flow of charge carriers from a surface or over a potential-energy barrier. This occurs because the thermal energy given to the carrier overcomes the binding potential, also known as work function of the metal. The charge carriers can be electrons or ions, and in older literature are sometimes referred to as "thermions". After emission, a charge will initially be left behind in the emitting region that is equal in magnitude and opposite in sign to the total charge emitted. But if the emitter is connected to a battery, then this charge left behind will be neutralized by charge supplied by the battery, as the emitted charge carriers move away from the emitter, and finally the emitter will be in the same state as it was before emission. The thermionic emission of electrons is also known as *thermal electron emission*.

The classical example of thermionic emission is the emission of electrons from a hot cathode, into a vacuum (archaically known as the **Edison effect**) in a vacuum tube. The hot cathode can be a metal filament, a coated metal filament, or a separate structure of metal or carbides or borides of transition metals. Vacuum emission from metals tends to become significant only for temperatures over 1000 K. The science dealing with this phenomenon has been known as **thermionics**, but this name seems to be gradually falling into disuse.

The term "thermionic emission" is now also used to refer to any thermally-excited charge emission process, even when the charge is emitted from one solid-state region into another. This process is crucially important in the operation of a variety of electronic devices and can be used for electricity generation (e.g., thermionic converter, electrodynamic tether) or cooling. The magnitude of the charge flow increases dramatically with increasing temperature.

## 5<sup>th</sup> topic

### Richardson's Law

In any solid metal, there are one or two electrons per atom that are free to move from atom to atom. This is sometimes collectively referred to as a "sea of electrons". Their velocities follow a statistical distribution, rather than being uniform, and occasionally an electron will have enough velocity to exit the metal without being pulled back in. The minimum amount of energy needed for an electron to leave a surface is called the work function. The work function is characteristic of the material and for most metals is on the order of several electron volts. Thermionic currents can be increased by decreasing the work function. This often-desired goal can be achieved by applying various oxide coatings to the wire.

In 1901 Richardson published the results of his experiments: the current from a heated wire seemed to depend exponentially on the temperature of the wire with a mathematical form similar to the Arrhenius equation. Later, he proposed that the emission law should have the mathematical form

$$J = A_G T^2 e^{-\frac{W}{kT}}$$

where  $J$  is the emission current density [SI unit: A/m<sup>2</sup>],  $T$  is the thermodynamic temperature of the metal [SI unit: kelvin (K)],  $W$  is the work function of the metal,  $k$  is the Boltzmann constant, and  $A_G$  is a parameter discussed next.

Taking the logarithm of both sides

$$\ln J = \ln A_G + 2 \ln T - \frac{W}{kT}$$

Thus, the equation showing the relationship between current densities at two temperatures is

$$\begin{aligned} \ln J_2 - \ln J_1 &= \ln A_G - \ln A_G + 2 \ln T_2 - 2 \ln T_1 + \frac{W}{kT_1} - \frac{W}{kT_2} \\ \ln \left( \frac{J_2}{J_1} \right) &= 2 \ln \left( \frac{T_2}{T_1} \right) + \frac{W}{k} \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \end{aligned}$$

In the period 1911 to 1930, as physical understanding of the behaviour of electrons in metals increased, various different theoretical expressions (based on different physical assumptions) were put forwards for  $A_G$ , by Richardson, Saul Dushman, Ralph H. Fowler, Arnold Sommerfeld and Lothar Wolfgang Nordheim. Over 60 years later, there is still no consensus amongst interested theoreticians as to what the precise form of the expression for  $A_G$  should be, but there is agreement that  $A_G$  must be written in the form

$$A_G = \lambda_R A_0$$

where  $\lambda_R$  is a material-specific correction factor that is typically of order 0.5, and  $A_0$  is a universal constant given by

$$A_0 = \frac{4\pi m k^2 e}{h^3} = 1.20173 \times 10^6 \text{ A m}^{-2} \text{ K}^{-2}$$

where  $m$  and  $-e$  are the mass and charge of an electron, and  $h$  is Planck's constant.

In fact, by about 1930 there was agreement that, due to the wave-like nature of electrons, some proportion  $r_{av}$  of the outgoing electrons would be reflected as they reached the emitter surface, so the emission current density would be reduced, and  $\lambda_R$  would have the value  $(1-r_{av})$ . Thus, one sometimes sees the thermionic emission equation written in the form

$$J = (1 - r_{av}) A_0 T^2 e^{\frac{-W}{kT}}$$

However, a modern theoretical treatment by Modinos assumes that the band-structure of the emitting material must also be taken into account. This would introduce a second correction factor  $\lambda_B$  into  $\lambda_R$ , giving  $A_G = \lambda_B(1 - r_{av})A_0$ . Experimental values for the "generalized" coefficient  $A_G$  are generally of the order of magnitude of  $A_0$ , but do differ significantly as between different emitting materials, and can differ as between different crystallographic faces of the same material. At least qualitatively, these experimental differences can be explained as due to differences in the value of  $\lambda_R$ .

Considerable confusion exists in the literature of this area because: (1) many sources do not distinguish between  $A_G$  and  $A_0$ , but just use the symbol  $A$  (and sometimes the name "Richardson constant") indiscriminately; (2) equations with and without the correction factor here denoted by  $\lambda_R$  are both given the same name; and (3) a variety of names exist for these equations, including "Richardson equation", "Dushman's equation", "Richardson-Dushman equation" and "Richard-Laue-Dushman equation". In the literature, the elementary equation is sometimes given in circumstances where the generalized equation would be more appropriate, and this in itself can cause confusion. To avoid misunderstandings, the meaning of any "A-like" symbol should always be explicitly defined in terms of the more fundamental quantities involved.

