Landauer's Erasure Principle and the Fermi Energy of Metals

P. R. Silva - Retired Associate Professor – Departamento de Física – ICEx – Universidade Federal de Minas Gerais – email: prsilvafis@gmail.com

Abstract

A minimization of a free energy inspired in the Landauer's erasure principle combined with alternatives treatments of the Brownian motion of the free electrons, is used as a means to derive the Fermi energy of metals. The obtained result differs from the usual one by a small discrepancy between the coefficients of the two versions of it, when expressed as a function of the density of free electrons, its mass and the Planck's constant.

1- Introduction

The Fermi energy of metals is usually determined by considering the conduction electrons as free particles living in a box, where the occupancy of the energy levels is done by taking in account the Pauli exclusion principle, reflecting the fermionic character of the charge carriers [1,2,3].

As a result, it is obtained the next relation for the Femi energy, E_F, in three dimensions

$$E_F = [\, h^{2} / (8\, m)]\, (3/\pi)^{2/3}\, n^{2/3}, \qquad (1)$$

where h is the Planck's constant, m the electron mass and n the density of conduction electrons.

2 – Landauer's erasure principle applied to metals

As was pointed out by Jacobs [4], Landauer's erasure principle [5] states that: whenever a single bit of information is erased, the entropy in the environment to which the information storing system is connected must increase at least $k_B \ln 2$, where k_B is the Boltzmann's constant. Meanwhile, a free electron in a metal travels in average a distance equal to its mean free path, with a constant velocity v_F, until to collide with the ionic vibrations (phonons). In the collision process, the free electron loses its memory.

To pursue further, we propose associate to the Fermi energy, E_F, a string of length equal to its Fermi wavelength, composed of unit cells having a size equal to the Compton wavelength of the electron. Next we introduce a quasi-particle with a mass-energy defined as

$$\mu c^2 = E_F v_F / c. \tag{2}$$

As can be seen from (2), this quasi-particle has a mass-energy given by its Fermi energy divided by the number of cells in the string. Defining

$$\Delta F = \Delta U - T\Delta S = \tfrac{1}{2} \mu c^2 - k_B T \ln 2, \tag{3}$$

where F, U and S are respectively the free and internal energies and the entropy, and T the temperature. The quasi-particle self interaction, leads to a variation in the internal energy equal to that of a particle of reduced mass $\frac{1}{2}\mu$. Making the requirement that

$$\Delta F|_{T=T^*} = 0, \tag{4}$$

yields to the relation

$$E_F^3 = (k_B T^*)^2 \, 2 \, (\ln 2)^2 \, m c^2. \tag{5}$$

2- Quantum mechanics and diffusion of the particles

Transport properties by free electrons in metals, occurs due to motion of free particles which suffers eventual collisions with the lattice vibrations (phonons). The time-dependent Schrodinger equation for a free particle in one-dimension, where a differential operator is applied the wave function Ψ, reads

$$i \hbar \, \partial\Psi / \partial t = - \hbar^2 / (2m) \Delta\Psi. \tag{6}$$

In this work we propose that the same recipe can be used to describe the evolution of the probability density $\Psi^*\Psi$, namely

$$i \hbar \, \partial(\Psi^*\Psi) / \partial t = - [\hbar^2 / (2m)] \partial^2(\Psi^*\Psi) / \partial x^2. \tag{7}$$

Performing averages on the two sides of (7), it is possible to write

$$\left| - [\hbar^2 / (2m)] \langle \partial^2(\Psi^*\Psi) / \partial x^2 \rangle \right| = [(2\hbar^2) / m] \langle \Psi^*\Psi \rangle / \ell^2. \tag{8A}$$

and

$$\left| \, i \hbar \, \partial \langle \Psi^* \Psi \rangle / \partial t \, \right| = 2 \hbar \langle \Psi^* \Psi \rangle / \tau. \qquad (8B)$$

In (8A) and (8B), ℓ and τ are respectively the characteristics length and time of the problem. Making the equality between the right hand sides of these relations leads to

$$\tau = m \, \ell^2 / \hbar. \qquad (9)$$

The above relation is the quantum analogous to the scaling relation of the Brownian motion.

4 – The density of charge carriers comes to the game

The density of charge carriers was estimated in a previous work [6].There, among other achievements, it was possible to deduce the Drude formula for the electrical conductivity, starting from the Landauer's relation [7] for the quantum conductance, based in the modern paradigm: "conduction is transmission" (please see also [8]). By now it is convenient to establish a link of the density of charge carriers with some characteristics lengths of the problem. It is well known clue that the electrical conductivity always happens in a regime of charge neutrality. In this way the number of scatter centers per unit of volume n, will be equal to the number density of the electrons of conduction.

By considering a cylinder shaped tube with longitudinal size equal to the electron mean free path λ and radius equal to the geometric average of ℓ_0 (the size of a typical channel of conduction) and ℓ_F (the reduced Fermi wavelength), it is possible to write

$$n \, \pi \, \ell_0 \, \ell_F \, \lambda = 1. \qquad (10)$$

But

$$\ell_F \, \lambda = \hbar \, \tau / m = \ell^2, \qquad (11)$$

where in obtaining the second equality, equation (9) was took in account. The information of (110 into (100 leads to

$$\tau = m / (n \, \pi \, \hbar \, \ell_0). \qquad (12)$$

The maximum value of the characteristic time happens when ℓ_0 is equal to the reduced Compton wavelength of the electron, namely $\ell_0 = \hbar/(mc)$. Using this into (12) yields

$$\tau_{max} = (m^2 c)/(n \pi \hbar^2). \quad (13)$$

Therefore we obtained a mean time between collisions which goes with the inverse of the density of charge carriers. Besides this, as was found in reference [6], this maximum characteristic time leads to the maximum conductivity of a metal in the diffusive regime.

5 – Evaluating the Fermi energy

The amount of thermal energy $k_B T^*$, which appears in eq.(5) can be thought as the energy of a ground state (vacuum) of a one-dimensional harmonic oscillator. In the appendix, the reasoning to this choice will better elaborate. To pursue further on this subject it is worth to write

$$k_B T^* = h/(2 \tau_{max}) = (n \pi \hbar^2 h)/(2 m^2 c). \quad (14)$$

Inserting (14) into (5) we get

$$E_{FN} = [(\ln 2)^2/(32 \pi^2)]^{1/3} (h^2/m) n^{2/3}, \quad (15)$$

where E_{FN} stands for the new Fermi energy deduced in this work, which must be compared with well known relation given by eq. (1).

In order to better compare the two relations for the three-dimensional Fermi energy of metals, it is convenient to write the approximated relations

$$E_{FN} \approx .1150 (h^2/m) n^{2/3}, \quad (15A)$$

$$E_F \approx .1212 (h^2/m) n^{2/3} . \quad (1A)$$

There is a five percent discrepancy between the numerical coefficients appearing in the above relations.

APPENDIX

The free particle model used in this work in order to describe the motion of the charge carriers through the whole crystal can be modified, perhaps leading to a more realistic picture of the transport phenomena in metals. This can be accomplished by considering a one-dimensional harmonic oscillator with a time-dependent spring constant k(t). Here as was done in

section 3, the Hamiltonian operator will be applied to the probability density function, instead to the wave function Ψ. To do this it is convenient to write

$$- [\hbar^2/(2m)]\, \partial^2(\Psi^*\Psi)/\partial x^2 + \tfrac{1}{2}\, k\, x^2\, (\Psi^*\Psi) = i\, \hbar\, \partial(\Psi^*\Psi)/\partial t. \qquad (A.1)$$

Proceeding as was done in section 3, performing averages and taking the absolute value of each term, we find

$$[\, \hbar^2/(m\, \ell^2)]\, \langle\Psi^*\Psi\rangle + \tfrac{1}{2}\, k\, \ell^2\, \langle\Psi^*\Psi\rangle = \hbar\, \langle\Psi^*\Psi\rangle/\tau. \qquad (A.2)$$

Dividing (A.2) for $\langle\Psi^*\Psi\rangle$ leads to the equation

$$\tfrac{1}{2}\, k\, \ell^4 - (\, \hbar/\tau)\, \ell^2 + \hbar^2/m = 0. \qquad (A.3)$$

Solving (A.3) for ℓ^2 yields

$$k\, \ell^2 = \hbar/\tau \pm [((\, \hbar/\tau)^2 - \hbar^2\, 2\, k(t)/m\,)^{1/2}. \qquad (A.4)$$

In the diffusion process undergone by the conduction electrons in metals, only in a very small fraction of the time of flight the electron interact with the lattice vibrations, which leads to the deviation of its original path. A way of representing this could be

$$\omega(t) = \pm(1/\tau)\, \cos(f\, t). \qquad (A.5)$$

In (A.5), the frequency $f >> 1/\tau$. Thus performing average over the high frequencies f, leads to

$$\langle\, \omega^2\, \rangle_f = \langle[\pm(1/\tau)\, \cos(f\, t)]^2\rangle_f = \tfrac{1}{2}\, (1/\tau\,)^2. \qquad (A.6)$$

Performing time-average over (A.4), and using (A.6) to evaluate the second term inside the radical, we have a cancellation of the radical and we get

$$2\pi\, \ell^2\, \langle\, k\, \rangle_f = A^2\, \langle\, k\, \rangle_f = h/\tau. \qquad (A.7)$$

In (A.7), $2\pi\,\ell^2$ was identified with the amplitude squared of a classical harmonic oscillator. By considering a characteristic temperature T*, it is thus possible to write

$$K_B T^* = h/(2\,\tau). \qquad \text{(A.8)}$$

The above result was used in section 5 of this work.

REFERENCES

[1] C. Kittel, Introduction to Solid State Physics, Fifth Edition, Wiley, 1976 - Ch. 6

[2] J. W. Rohlf, Modern Physics from α to Z^0, Wiley, 1994 – Ch. 14

[3] P. A. Tipler, Modern Physics, Worth Publishers, 1978 – Ch. 9

[4] K. Jacobs, arXiv: quant-ph/0512105v1 (Dec. 2005)

[5] R. Landauer, IBM J. Res. Develop.**5**, 183(1961)

[6] P. R. Silva, Marcos Sampaio, C. Nassif, M. C. Nemes, Phys. Lett. A **358**, 358(2006)

[7] R. Landauer, IBM J. Res. Develop. **1**, 223(1957)

[8] Y. Imry and R. Landauer, Rev. Mod. Phys. **71**, S306, Centenary(1999)