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### Theoretical aspects of Microwave Frequency Transport in Generic Dimensionality Semiconductors

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# Summary

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\* Original elaboration of this work. A marked section extends the mark to the related subsections.

# Introduction

The present work can be classified as an investigation for the theoretical study of semiconductors in the microwave ( $\mu$ w) frequency domain. This range owns two properties that let it to be a hot subject for the next years: from one side, there is a basic need of such a characterization to get a satisfactory description of the fundamental solid state physics; from the other side there is the urgent need to analyze and increase performances of technological products in order to improve the quality of services in human life and business. IBM announced in March 2002 the realization of the fastest silicon-based transistor, by using a modified design of a heterojunction bipolar transistor (HBT) and SiGe technology, working at a speed of 210 GHz. New methods to allow contactless measurements techniques of the transport properties of semiconductors are needed for a  $\mu$ w characterization to cover the whole range.

This work presents and analyzes some results about the theoretical relationship between the electrical transport and the frequency effects, when the currents are excited by the coupling to a millimeter and sub-millimeter electromagnetic field. The first chapter evidences the way both to describe the transport properties at generic dimensionality and to predict qualitatively different behavior in low-dimensional systems. The second chapter describes the extension of the analytical treatment of the Hall mobility and the Hall factor to the microwave<sup>•</sup> ( $\mu$ w) excitation case. In particular, scattering-independent calculations are analyzed. The third chapter reports principal 2D and 3D scattering mechanism properties and shows the application of the results obtained in the second chapter by using the scattering information in some interesting physical cases. The fourth chapter describes, from the most general theoretical approach, a supersymmetric Lagrangian model governing a disordered system and the microwave-infrared (IR) *d*-dimensional conductivity by taking into account the impurities present in a crystal.

The work covers a part of the Ph.D. thesis realized under the supervision of Prof. Massimo Martinelli (IPCF – CNR, Pisa, Italy) and discussed at the Physics Department of the University of Pisa in October 2002.

<sup>•</sup> The microwave frequency domain spans the electromagnetic spectrum between  $10^{10}$  and  $10^{12}$  Hz. Another common classification based on the wavelenght distinguish' the millimetre (from  $3 \cdot 10^{10}$  to  $3 \cdot 10^{11}$  Hz) and submillimetre (from  $3 \cdot 10^{11}$  to  $3 \cdot 10^{12}$  Hz) waves inside of this range.

### **1** Effects of dimensionality in solids

This chapter introduces some arguments to show the effects of the dimensionality in a particle ensemble like carriers in a solid, depending essentially on the quantum nature of the treatment. The transport of carriers in crystals is usually described by the Boltzmann equation. This is possible when temperature regime and fluctuations due to disorder are not relevant. When the disorder increases or the temperature decreases, the system is described by the Schroëdinger equation including an averaged random potential. For this reason an analytical study results quite difficult and solutions can be derived only in approximated schemes. Generally speaking, a system shows relevant fluctuations if the thicknesses of a crystal along some directions reach the scale of scattering length. In other words, it happens that the physical dimensionality of the system is lowered and the paths of carriers have a greater probability to interfere on themselves [EFE95]. There is a deep connection between transport in such crystals and critical phenomena; after the scaling conjecture of Thouless in 1977, Abrahams, Anderson, Licciardello and Ramakrishnan proposed a simple argument to explain metal-insulator Anderson transition in 1979. The most general bridge between transport theory and quantum field theory and critical phenomena consists in the identification of supersymmetry as a physical symmetry of the lagrangian expression for a disordered system and is due to Efetov ('80), and will be briefly discussed in Chapter 4.

In this Chapter is analyzed the  $\mu$ w-IR frequency transport in semiconductors at a generic dimensionality and a qualitative argument explaining the metal-insulator transition is suggested. This result is connected to the shape of the density of states (DOS) analytical continuation derived in a quantum mechanical picture. The relativistic extension is also derived in Appendix A. The supersymmetry principle derivation is proposed at the end of this work. The first and the fourth chapter both give the deviation of the  $\mu$ w and the IR conductivity from the d.c.

# **1.1 Qualitative picture of quantum corrections at low dimensionality**

In a weak disorder picture, the interaction between carriers and defects is considered as a scattering of periodic Bloch waves on impurity centers [ZIM69, par. 7.4]. In the classical limit it leads to the Boltzmann equation giving

$$\sigma_{0} = \frac{n e^{2} \tau}{m^{*}} \tag{1.1}$$

where *e* is the electron charge, *n* is the electronic density in a unit of volume of the metal,  $m^*$  is the effective electron mass and  $\tau$  is the *scattering* time, depending on mechanisms of collision of carriers. According to the concentration of impurities, the crystalline material can vary from a good

metal behavior to that of an insulator when disorder becomes sufficiently strong. The equation above is no longer valid in this picture and the proper description must be fully based on quantum mechanics. In a metal the eigenfunctions at eigenenergy near to Fermi level are extended over the sample, but in the insulating regime the electron wave function can become localized and it decays exponentially from the impurity.

Chronologically, the derivation of the argument of Khmelnitskii [ALT83] follows the scaling argument of Abrahams *et al.* [ABR79] but it is more useful to consider the first one to evaluate the weight of quantum correction at low dimensionality as a starting point.



Figure 1.a) Paths without intersections from the point  $r_1$  to the point  $r_2$ ; b)self-interacting path [EFE95].

When considering the probability to reach the point  $r_2$  from  $r_1$  (Figure 1.a-b), following elementary quantum mechanics the total probability is not the sum of all probabilities of the paths  $W_i$ , but, if  $A_i$  are the complex amplitudes:

$$W = \left| \sum_{i} A_{i} \right| = \sum_{i} \left| A_{i} \right|^{2} + \sum_{i,j} \left| A_{i} A_{j}^{*} \right|^{2}$$
(1.2)

The first term corresponds to the sum of the contribution of each path, while the second to the interference among all paths. In effect the contribution of the interference among different paths oscillates very fast and it can be neglected [EFE95]. The behavior of self-interacting paths is different. A qualitative deep difference is due to the probability of a path to pass twice in the same point: at d = 3 this probability is extremely small with respect to unit, but at d = 1,2 it is a unit. This allows to calculate quantum deviations from  $\sigma_0$  at generic dimensionality, such that [GOR79]:

$$\frac{\Delta\sigma}{\sigma_0} \propto -\int_{\tau}^{\tau_{\varphi}} dt \nu \lambda^{d-1} (D_0 t)^{-d/2}$$
(1.3)

where  $\tau$  is the elastic scattering time (there is no contribution when *t* is lower than the scattering time),  $\tau_{\varphi}$  is the inelastic scattering time (tends to infinity when temperature *T* goes to zero), *v* the velocity of a carrier,  $\lambda \sim h/2\pi p$  the scattering length related to the momentum of the carrier, and  $D_0$  is the classical diffusion coefficient:

$$D_0 = \frac{v_F^2 \tau}{d} \tag{1.4}$$

This effect is called weak localization because the decrease of conductivity can be considered as a precursor of localization.

# **1.2 Density Of States at a generic dimensionality and DOS argument for metal-insulator transitions\***

There is a second effect depending on dimensionality that concerns collective properties of carriers. Since carriers are fermions, they cannot hold the same quantum numbers. For each energy only two electrons with opposite spin projection along an axis can exist at the same time. The consequence is that all the states up to ones at Fermi energy are filled at T = 0, and a basic information of the system

is how many levels at the same energy are allowed provided that many sets of values in momentum space can give the same energy for a carrier. Generally the density of states is calculated for a box or by using periodic boundary conditions and it can be found [KEL95] that the number of states at a certain energy is at various dimensionalities proportional to:

$$\left. dn(E) \right|_{d=1} \propto \frac{dE}{\sqrt{E}} \tag{1.5}$$

$$\left. dn(E) \right|_{d=2} \propto dE \tag{1.6}$$

$$\left. dn(E) \right|_{d=3} \propto \sqrt{E} dE \tag{1.7}$$

In order to explain qualitative different behavior between 3D and lower dimensionality systems, it is useful to consider the analytical continuation at d dimensions of the most general expression of DOS. By imposing a heuristic quantization, since along each direction i in a box having thickness L the periodic boundary condition gives:

$$p_i = \eta k_i = \frac{n_i h}{2L} \tag{1.8}$$

it is possible to evaluate:

$$dn = \prod_{i}^{d} dn_{i} = \left(\frac{h}{2L}\right)^{-d} d^{d} p = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})} \left(\frac{h}{2L}\right)^{-d} p^{d-1} dp$$
(1.9)

The last transformation involves a factor representing the hypervolume of a *d*-dimensional sphere. This volume has to be reduced by a factor  $2^d$  since it concerns the occupation in a momenta space. By using the non relativistic expression:

$$p = \sqrt{2mE} \rightarrow dp = \frac{1}{2}\sqrt{\frac{2m}{E}}dE$$
 (1.10)

the substitution gives:

$$dn = g(E)dE = \frac{\pi^{\frac{d}{2}}}{2^{d} \Gamma(\frac{d}{2})} \left(\frac{h}{2L}\right)^{-d} (2m)^{\frac{d}{2}} E^{\frac{d-2}{2}} dE$$
(1.11)

Including spin degeneracy for particles with spin s:

$$g(E) = (2s+1)\frac{\pi^{\frac{d}{2}}}{2^{d} \Gamma(\frac{d}{2})} \left(\frac{2L}{h}\right)^{d} (2m)^{\frac{d}{2}} E^{\frac{d-2}{2}}$$
(1.12)

Restricting the attention only on the functional part depending on the energy, the plot of DOS versus the energy and the dimensionality (Figure 1.c) shows that decreasing from 3D to 2D the preferred states of the system switch from high energy to low energy (low momentum, localized states). This effect becomes stronger at lower dimensionality, as 1D and 0D. The transition from a 3D behavior to a 2D one can be viewed as a critical realization of low energy states by allowing a sudden change of energy in a certain number of carriers. At the same time a compression of the number of states occurs at higher energy: this can be interpreted by a re-arrangement of carriers, which requires energy.



Figure 1.c. The analytical continuation of density of states shows a qualitatively different behavior above and under the 2D case. This can be considered as argument suggesting possible localization at integer dimensionality lower that 3.

In the Appendix A it is reported the correspondent DOS of the relativistic electron gas.

### 1.3 An application: quantum rings\*

There is a case where a periodic boundary condition is physically fulfilled i.e. in quantum rings. The DOS is the same of previous paragraph in 1D case, except that L is substituted by  $2\pi R$  where R is the radius of the ring, so:

$$dn(E)\Big|_{ring} = \left(2s+1\right)\frac{R}{h}\sqrt{\frac{2m}{E}}dE$$
(1.13)

The interesting fact is that the physical cutoff usually imposed in compact geometry systems changes. In general when integrating on momentum divergences are frequently present. At the same time equations do not lose their validity in force of physical limitations on momentum admitted values.

There are two limits to impose to the inverse of momentum provided by the maximum length in the system along an axis *L* and the minimum physical length i.e.  $\lambda$  the mean free path [RID95]. To give an example,  $\lambda$  is of the order of 20nm in 3D degenerate semiconductors [RID95]. In other terms:

$$\frac{1}{L} < k < \frac{1}{\lambda} \tag{1.14}$$

and the great number of states at low energy allowed by DOS is only partially filled. In quantum rings the condition on the length of the sample does not act because there are only carriers interfering constructively with themselves. There is no limit in the maximum length of the system and 1/L tends to 0 so that in principle all the energy states may be filled because:

$$0 < k < \frac{1}{\lambda} \tag{1.15}$$

In practice a total removal of a lower limit for momenta is not reasonable because of the structure of DOS, which diverges at low energy. A new cutoff can be considered remembering that fluctuations in energy are due to:

$$\Delta E > \frac{\eta}{\tau} \tag{1.16}$$

where  $\tau$  is the life of carrier between two scatterings. Defects in crystals destroy in any case coherence at a certain level.

# **1.4 Scaling hypothesis in metal-insulator transition and diffusion modes**

In 1979 Abrahams, Anderson, Licciardello and Ramakrishnan proposed a formal description by a scaling hypothesis, expressing Thouless hypothesis that the only quantity determining the behavior of the system is the resistivity [THO77, ABR79]. They described a disordered metal in an arbitrary dimension *d* combining  $b^d$  cubes of size *L* into blocks of the size *bL*. If the conductance *g* (the inverse of the resistivity) is the only parameter determining the phase of the system, this gives:

$$g(bL) = f(b, g(L))$$
 (1.17)

where f is an unknown function. Taking the limit  $b \rightarrow 1$  the differential form is:

$$\frac{d\ln g(L)}{d\ln L} = \beta(g(L)) \tag{1.18}$$

where the logarithmic derivative extracts the power behavior with respect to *L*. It is formally not possible to calculate the function  $\beta$ , but its asymptotes may be evaluated. For large *g* one can use the classical expression  $g(L) = \sigma_0 L^{d-2}$  so:

$$\beta(g) = d - 2 \tag{1.19}$$

When g is small, the localization is surely valid and g falls off exponentially  $g(L) = g_0 e^{-\alpha L}$  so:

$$\beta(g) = \ln \frac{g}{g_0} \tag{1.20}$$

The behavior of the  $\beta$  function strongly depends on the dimensionality of the space as represented in the Figure 1.d. At d = 3 this function must vanish somewhere and an unstable fixed point  $g_c$  [LEB91, ZIN89] exists where  $\beta$  turns to zero. At this point the conductance g does not change in the size of the sample and this corresponds to the point of the Anderson metal-insulator transition.

At d = 1, it holds  $\beta < 0$  for any disorder, provided that it is smooth and monotonous, and this agrees with prediction for wires and chains. At d = 2 it is also everywhere negative, indicating a localization. This last result has been confirmed numerically by more complex treatments substituting the one-parameter scaling by a distribution function of conductances [ALT85].



Figure 1.d Plot of  $\beta(g)$  versus ln g for d < 2, d = 2, d > 2; g(L) is the conductance [EFE95].

This showed a qualitative difference between spaces at different dimensionality and it was the starting point to a quantum perturbation theory providing quantitative predictions. Imposing the equation for an electron gas by an opportune Hamiltonian does it. In particular this operator contains a random potential describing the impurities in crystals:

$$H\psi_{k} = \left(H_{0} + H_{I}\right)\psi_{k} = \left(\frac{p^{2}}{2m} + u(r)\right)\psi_{k} = E_{k}\psi_{k}$$
(1.21)

in the simplest case, where impurities do not act on the spin and:

$$\langle u(\hat{F}) \rangle = 0$$

$$\langle u(\hat{F})u(\hat{F}') \rangle = \frac{1}{2\pi\nu\tau} \delta(\hat{F} - \hat{F}')$$
(1.22)

with  $\tau$  the mean free time. It is not possible to solve analytically this equation for an arbitrary potential. Fortunately one is interested in statistical properties only: it is useful to consider averaged quantities and it can be done a diagrammatic expansion. Families of diagrams constitute diffusion modes, and the theory is based on solving the system by finding the Green function and calculating from this the physical quantities such as the conductivity. This procedure led to investigate successfully in '80 mesoscopic phenomena and found experimental confirmations.

Unfortunately it works only when the quantum effects are weak and the properties of the system are almost classical. By increasing disorder the Anderson transition is reached and the system switch to an insulating phase, where perturbation theory is no longer valid. Where localization is possible the diagrammatic approach does not work. The perturbative approach is substituted by the supersymmetric one, that covers the results obtained by this theory but is the only method to obtain energy level statistics, quantum size effects, mesoscopics [EFE97]. This is shortly described in the Chapter 4.

### 2 Microwave Hall Mobility

In this chapter the interest is devoted to the evaluation of the frequency dependence of mobility, starting from quantum mechanics principles. This allows determining the quantity corresponding to the Hall factor versus both the cyclotron frequency, as usually done, and the  $\mu$ w frequency of electrons interacting with an electromagnetic wave. The analysis is, for the moment, devoted to obtain results where the dependence of the scattering time with respect of the energy is implicit. The scattering mechanism will be included in the next chapter.

The simplest theory that describes the scattering effects is the Drude model:

$$\sigma(\omega) = \frac{n_e e^2 \tau}{m} \frac{1}{1 - i\omega\tau}$$
(2.1)

where  $n_e$  is the electron density and *m* the electron mass. The regime defined by the condition  $\omega \tau \ll 1$  is called Hagen-Rubens limit. The opposite limit is when  $\omega \tau \gg 1$  and it is called the relaxation limit [KLE93].

### 2.1 Hall mobility as a function of frequency

By considering an electric field applied to a semiconductor, without loss of generality, it can be supposed that this contains only free charges. An enough low concentration allows us to neglect the interaction between themselves and the effects of the local field on ionic charges.

In an *n*-doped semiconductor, if  $\Phi$  is the electric potential of the applied field, the time evolution equation of the electron is in c.g.s.:

$$(\mathbf{H}_{0} - e\Phi)\psi(\mathbf{r}, t) = i\eta \frac{\partial\psi}{\partial t}$$
(2.2a)

where  $H_0$  is the monoelectronic Hamiltonian of the electron in lattice in absence of external perturbations, *e* is the electric charge and  $\psi$  the wave function of the electron respectively. Let's consider the electric potential varying slowly as a function of **r**, the equation becomes, for the envelope functions [CAR96]:

$$\left[\mathsf{E}_{c}(0) - \left(\frac{\eta}{2m^{*}}\right)\frac{\partial^{2}}{\partial \mathbf{R}^{2}} - e\Phi(\mathbf{R})\right]C(\mathbf{R}, t) \approx i\eta\frac{\partial}{\partial t}C(\mathbf{R}, t)$$
(2.2b)

This leads, in a quasi-classical scheme, to the following equation for the electron, changing its mass by the effective one  $m^*$ :

$$m^* \frac{d^2 \mathbf{r}}{dt^2} + \frac{m^*}{\tau} \left( \frac{d \mathbf{r}}{dt} \right) = -e \left( \mathbf{E} + \frac{d \mathbf{r}}{dt} \times \mathbf{B} \right)$$
(2.3)

where **E** and **B** are the applied fields and  $\tau$  the scattering constant. A necessary hypothesis is that the electron is confined in a parabolic band, and intraband transitions are forbidden; from the energy point of view, it is needed that the applied field is weak, that is:

$$eEa_0 \ll \frac{\left[\Delta \mathsf{E}(\mathbf{k})\right]^2}{\mathsf{E}_{\mathrm{F}}} \tag{2.4}$$

where  $\Delta E(\mathbf{k})$  is the difference in energy between two contiguous bands at momentum  $\mathbf{k}$ ,  $a_0$  the lattice spacing and  $E_F$  is the Fermi energy of electron [ASC76]. Notice that the hypotheses of high disorder or low temperature are excluded by this treatment.

In the general case of a non-static electric field and a static magnetic field on the orthogonal axis,

$$\mathbf{E} = \begin{pmatrix} E_x \\ E_y \\ 0 \end{pmatrix} e^{i\omega t} \qquad \mathbf{B} = \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix}$$
(2.5)

solving the Eq. (1.2.1) the current and the conductivity tensor can be written as:

$$\begin{pmatrix} j_x \\ j_y \end{pmatrix} = n(-e) \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \begin{pmatrix} \sigma_0 & \sigma_1 \\ -\sigma_1 & \sigma_0 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix} =$$

$$= \frac{\frac{ne^2}{m^*}}{\left(j\omega + \frac{1}{\tau}\right)^2 + \left(\frac{eB}{m^*}\right)^2} \begin{pmatrix} j\omega + \frac{1}{\tau} & -\frac{eB}{m^*} \\ \frac{eB}{m^*} & j\omega + \frac{1}{\tau} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix}$$
(2.6)

When  $\omega \tau \ll 1$  (for example for a semiconductor having a scattering time of the order of  $10^{-12}$  sec, the upper limit is  $\omega = 10^{11}$ Hz rad) one can reach the same conclusion of the static case and has the **Hall mobility**:

$$\mu_{H} = \frac{1}{B} \frac{|\sigma_{1}|}{Re \,\sigma_{0}} \cong \mu_{0} \tag{2.7}$$

It is in the general case mandatory to consider a mean value on the energy distribution, remembering that  $\tau = \tau(E)$ , so you have the expression of the diagonal and off-diagonal conductivity [WAT61]:

$$\left\langle \sigma_{0} \right\rangle = \frac{ne^{2}}{m^{*}} \left\langle \frac{\tau \left( j\omega\tau + 1 \right)}{\left( j\omega\tau + 1 \right)^{2} + \left( \omega_{c}\tau \right)^{2}} \right\rangle$$
(2.8)

$$\left\langle \sigma_{1} \right\rangle = -\frac{ne^{2}}{m^{*}} \left\langle \frac{\omega_{c} \tau^{2}}{\left(j\omega\tau + 1\right)^{2} + \left(\omega_{c}\tau\right)^{2}} \right\rangle$$
(2.9)

and, for the mobility:

$$\mu_{H} = \frac{1}{B} \frac{\left| \left\langle \sigma_{1} \right\rangle \right|}{Re \left\langle \sigma_{0} \right\rangle} \tag{2.10}$$

where:

$$\omega_c = \frac{eB}{m^*} \tag{2.11}$$

#### is the cyclotron frequency.

The mobility is in general a non-diagonal tensor and the expression between static mobility and Hall mobility changes at frequencies such that  $\omega \tau \approx 1$  and greater values. In fact (2.7) is no longer valid and it should be interesting to evaluate the difference between static, Hall and Microwave Hall mobility.

#### 2.2 $\mu$ w mobility equation in low magnetic field\*

In this section the interest is for the explicit derivation of the effects due to the non-vanishing frequency dependence when the diagonal and off-diagonal conductivities appearing in the Hall mobility are averaged. This analysis looks at the  $\mu w$  effects and not to consequences of a high magnetic field. The limit where the following equations are carried out is for:

$$(\omega_c \tau)^2 \ll \operatorname{Re}\left[(1+j\omega\tau)^2\right]$$
(2.12)

where Re indicates the real part. In this limit, the Eq. (2.8-9) become:

$$\left\langle \sigma_{0} \right\rangle = \frac{ne^{2}}{m^{*}} \left\langle \frac{\tau}{1+j\omega\tau} \right\rangle = \frac{ne^{2}}{m^{*}} \left\langle \frac{\tau}{1+\omega^{2}\tau^{2}} \left(1-j\omega\tau\right) \right\rangle$$
(2.13)

$$\left\langle \sigma_{1} \right\rangle = -\frac{ne^{2}}{m^{*}} \left\langle \frac{\omega_{c} \tau^{2}}{\left(1 + j\omega\tau\right)^{2}} \right\rangle = -\frac{ne^{2}}{m^{*}} \left\langle \frac{\omega_{c} \tau^{2}}{\left(1 + \omega^{2}\tau^{2}\right)^{2}} \left(1 - \omega^{2}\tau^{2} - 2j\omega\tau\right) \right\rangle$$
(2.14)

The equation (2.10) of mobility contains the real part of the average diagonal conductivity, so the interest focuses on:

$$\operatorname{Re}[\langle \sigma_0 \rangle] = \frac{ne^2}{m^*} \left\langle \frac{\tau}{1 + \omega^2 \tau^2} \right\rangle$$
(2.15)

The off diagonal conductivity is also a complex quantity. Although this, for a low-loss material, a mobility measurement get out the real part of it, while the imaginary part contributes to the real part of the dielectric constant. The justification comes from Appendix B and the evaluation gives:

$$\varepsilon''(\omega) = \frac{4\pi ne \ \mu'(\omega)\omega'}{\left|\omega\right|^2} \tag{2.16}$$

where indexes refer to the real and the imaginary part of the quantities following z = z' + iz''. This shows that for our purpose is sufficient to consider the real part of the mobility. For sake of simplicity **the real part of the mobility will be called**  $\mu$  **instead of**  $\mu'$ . The quantity to be averaged is then:

$$\left\langle \sigma_{1} \right\rangle = -\frac{ne^{2}}{m^{*}} \left\langle \frac{\omega_{c} \tau^{2}}{\left(1 + \omega^{2} \tau^{2}\right)^{2}} \left(1 - \omega^{2} \tau^{2}\right) \right\rangle$$
(2.17)

so that the  $\mu$ w Hall mobility to be measured, excluding its imaginary part which is included in real part of the dielectric constant, in the low magnetic field limit, is:

$$\mu_{H} = \frac{1}{B} \frac{\left| \operatorname{Re}\langle \sigma_{1} \rangle \right|}{\operatorname{Re}\langle \sigma_{0} \rangle} = \frac{\left\langle \frac{\omega_{c} \tau^{2}}{\left( 1 + \omega^{2} \tau^{2} \right)^{2}} \left( 1 - \omega^{2} \tau^{2} \right) \right\rangle}{B \left\langle \frac{\tau}{1 + \omega^{2} \tau^{2}} \right\rangle}$$
(2.18)

It is interesting that by increasing the  $\mu w$  applied field the averaged quantity vanishes for some values of the energy such that:

$$\tau(E) = \omega^{-1} \tag{2.19}$$

The existence of this point is granted by the monotonic behavior in energy of the scattering time. Supposing that this derivation applies for example to a material having no energy dependence on the scattering time or eventually a (highly doped) degenerate semiconductor where density function is peaked at the Fermi energy [SMI78]:

$$\tau = \omega^{-1} \tag{2.20}$$

The absence of the cyclotron frequency at high frequency may be fatal to have correct results. For this reason it is necessary to evaluate the mobility in a no approximation scheme if  $\omega \tau$  is wanted to be of the order of unit.

### 2.3 General implicit $\mu$ w mobility equation for semiconductors\*

Here it is implicitly written the  $\mu w$  mobility in its most general form. This calculation involves the average with respect to the energy spectrum so it cannot be evaluated explicitly in general since every scattering mechanism shows a particular power dependence of scattering time versus the energy and a fully analytical solution is not known. Each scattering mechanism has to be evaluated separately. The real part of the mobility depends on the ratio between:

$$\operatorname{Re}\langle\sigma_{0}\rangle = \operatorname{Re}\left[\left\langle\frac{ne^{2}}{m^{*}}\frac{\tau\left(1+j\omega\tau\right)}{\left(j\omega\tau+1\right)^{2}+\left(\omega_{c}\tau\right)^{2}}\right\rangle\right] = \left\langle\frac{ne^{2}}{m^{*}}\frac{\tau\left[1+\left(\omega_{c}^{2}+\omega^{2}\right)\tau^{2}\right]}{\left[1+\left(\omega_{c}^{2}-\omega^{2}\right)\tau^{2}\right]^{2}+4\omega^{2}\tau^{2}}\right\rangle$$
(2.21)

$$\left|\operatorname{Re}\langle\sigma_{1}\rangle\right| = \operatorname{Re}\left[\left\langle\frac{ne^{2}}{m^{*}}\frac{\omega_{c}\tau^{2}}{\left(j\omega\tau+1\right)^{2}+\left(\omega_{c}\tau\right)^{2}}\right\rangle\right] = \left\langle\frac{ne^{2}}{m^{*}}\frac{\omega_{c}\tau^{2}\left[1+\left(\omega_{c}^{2}-\omega^{2}\right)\tau^{2}\right]}{\left[1+\left(\omega_{c}^{2}-\omega^{2}\right)\tau^{2}\right]^{2}+4\omega^{2}\tau^{2}}\right\rangle$$
(2.22)

This leads to:

$$\mu_{\rm H} = \frac{1}{\rm B} \frac{|{\rm Re}\,\sigma_1|}{{\rm Re}\,\sigma_0} = \frac{\left\langle \frac{\omega_c \tau^2 \left[1 + (\omega_c^2 - \omega^2)\tau^2\right]}{\left[1 + (\omega_c^2 - \omega^2)\tau^2\right]^2 + 4\omega^2\tau^2\right\rangle} \right\rangle}{B\left\langle \frac{\tau \left[1 + (\omega_c^2 + \omega^2)\tau^2\right]}{\left[1 + (\omega_c^2 - \omega^2)\tau^2\right]^2 + 4\omega^2\tau^2\right\rangle} \right\rangle}$$
(2.23)

The evaluation of this quantity is in general quite complex. Where possible, the evaluation of this expression will be done under the weak field approximation like Eq. (2.18).

# **3** Microwaves and scattering mechanisms

The aim of this section is the evaluation of the effect of the microwaves on the semiconductor transport by an examination of the dependence of the scattering time versus the energy for some scattering mechanism. The most general expression for scattering time is:

$$\frac{1}{\tau} = \frac{2\pi}{\eta} \sum_{\mathbf{q}} \left| M_{\mathbf{q}} \right|^2 \delta \left( \frac{p^2}{2m} - \frac{(\mathbf{p} - \mathbf{q})^2}{2m} \right) \frac{\mathbf{p} \cdot \mathbf{q}}{p^2}$$
(3.1)

where  $M_q$  is the scattering matrix element, **p** is the momentum of the carrier, **q** are the possible momentum transfers and *m* the equivalent mass.

Depending on different kind of scattering, the function  $M_q$  may behave in different ways versus the energy or the mass. The calculations are reported in texts as [RID88] and it must be considered the distinction between 2D and 3D semiconducting materials.

There are here in particular explicitly evaluated the  $\mu$ w phonon, alloy and ionized impurity scattering dependence versus the frequency in two-dimensional semiconductors. The first and the second does not require the average on the energy, while the latter does. The Figure 3 shows principal scattering mechanisms in 2DEGs.



Figure 3 The principal scattering mechanisms in 2DEGs. This applies in the HEMT family.

### **3.1 Scattering classification of bulk semiconductors**

For bulk semiconductors it is possible to outline a table to display the mass and temperature power dependences of the relaxation time  $\tau$  and the mobility  $\mu$  [LOO89]. Different dependencies are reported in Table 3.1.

	Relaxation Time		Mobility	
Mechanism	Energy	Mass	Energy	Mass
(1) Impurity				
(a) Ionized	3/2	1/2	3/2	-1/2
(b) Neutral	0	1	0	0
(2) Acoustic Phonon				
(a) Deformation	-1/2	-3/2	-3/2	-5/2
(b) Piezoelectric	1/2	1/2	-1/2	-3/2
(3) Optical Phonon				
(a) Polar	~1/2	-1/2	-	-3/2
(b) Non Polar	~-1/2	-3/2	-3/2*	-5/2
(4) Localized Potential				
(a) Alloy	-1/2	-3/2	-1/2	-5/2
(b) Space Charge	-1/2	1/2	-1/2	-1/2
(c) Barrier	-1/2	-3/2	-1/2	-5/2
(d) Well	-1/2	3/2	-1/2	1/2
(5) Dipole	1/2	-1/2	1/2	-3/2

\* KT being much lower than  $h\omega/2\pi$ .

Table 3.1. Mass and temperature dependencies of  $\tau$  and  $\mu$  for non-degenerate electrons.

### **3.2 Scattering classification of 2D semiconductors**

In two-dimensional systems the scattering mechanisms may differ from those in bulk semiconductors. Principally there can be considered four different mechanisms, which are of major importance in two-dimensional semiconductors: scattering by ionized impurities, phonon scattering, alloy scattering and surface (at interface) scattering. The latter occurs only in two-dimensional systems, while the others change from bulk semiconductors for some specific features, needing therefore special considerations [SHI98].

A general result that can be obtained is that for the same scattering mechanism the **relaxation time** in a two-dimensional layer is less than in a bulk sample and decreases by decreasing the layer thickness [SHI98]. Furthermore it acquires a factor proportional to  $\sim T^{1/2}$ . Defining *a* as the 2D sample thickness, *p* the momentum and  $\gamma$  a numerical factor of the order of a unit, it holds:

$$\frac{\tau_2}{\tau_3} = \gamma \frac{pa}{\eta} \tag{3.2}$$

Here it follows a list of the principal effects in main scattering mechanisms.

**Ionized impurities scattering**. The main difference from 3D scattering is due to different space distributions of scattering centers. They are usually ions, located at some distance from the layer plane; in modulation-doped heterostructures they are intentionally removed from the 2DEG plane so the mobility is governed not only by the concentration but also by the space distribution of the ions. It can be found that  $\tau$ ~E when a single subband is occupied.

**Phonon scattering**. The phonon spectrum is assumed to be the same as in bulk semiconductors;  $\tau$  is constant with respect to energy:  $\tau$ -const.

Alloy scattering. It appears only in alloys and is due to the random distribution of ions of the two elements and the local alloy composition. This is a short range potential, and it can be considered as a sum of  $\delta$  functions. It is noticeable in heterostructures where a narrow gap semiconductor containing the majority of carriers is an alloy rather than a pure chemical substance.  $\tau$  is constant with respect to the energy ( $\tau$ -const).

**Surface (interface) scattering**. It is caused by the non-ideal nature of the potential walls confining the carrier motion in a quantum well.

### **3.3 Scattering mechanisms in the triangular quantum well**

In actual devices the scattering mechanisms do not limit the high frequency response but they have strong effect on the mobility of the 2-DEG. The carriers lie within an undoped semiconductor triangular quantum well. The original undoped GaAs channel has been substituted by an InGaAs one with a thickness of tens of Å because the superior response of electrons in such alloy. This configuration let the quantum well be away from ionized impurities, necessary to have extra charge confined in the 2DEG. In a GaAs or InGaAs channel based structure, impurities are in the AlGaAs layers put under and above it. The high concentration of the carriers, when they are transported in the direction parallel to the heterointerface, let them to suffer negligibly from the effect of Coulomb scattering. The limitations to the carrier mobility in modulation-doped heterostructures are set by the interaction of electrons and the crystal lattice that undergoes vibrations due to finite temperature. In general residual background impurities are less than  $10^{14}$  cm<sup>-2</sup>, but the interaction with phonons cannot be screened. In GaAs, below 50 K, the polar optical phonons drops off and the mobility is dominated by piezoelectric interaction.

In a HEMT (High Electron Mobility Transistor), when the channel carrier density is reduced (by negative gate voltage), the mobility falls rapidly. This is an evidence of the reduction of electrostatic screening of the impurities due to lowering of concentration of electrons [ALI91].

This information completes the picture to focus the attention on some interesting case and to understand the behaviors of principal physical quantities to get out a quantitative analysis of  $\mu w$  average effects on the mobility.

# **3.4 2D and 3D averages in energy distribution of physical quantities**

In this paragraph the interest is to recall some familiar results that will be applied in the explicit analysis for scattering kinds.

The average of a physical quantity has to be performed by using a probability density distribution. In principle it can be thought that this function is the energy distribution of carriers, but this is true except for a further factor to multiply the distribution, due to the occupation of energy levels. In lack of this factor the analysis does not take account of the fact that the occupation of neighboring states will prevent transitions to them [BRO55]. The recognized form to express this average for spherical constant energy surfaces is:

$$\langle \varphi(E) \rangle = \frac{\int \varphi(E) EN(E) e^{-E/KT} dE}{\int EN(E) e^{-E/KT} dE}$$
(3.3)

where N(E) is the probability density function on the non-degenerate case and the *E* factor is due to effect discussed by [BRO55].

In general the scattering time is linked to the energy by:

if:

$$\tau = aE^{-s} \tag{3.4}$$

- The semiconductor is not in degenerate regime.
- a = a(T)

Before explicit scattering calculation, it may be useful to evaluate the normalization factor of the 2D and 3D cases. The constant factor due to DOS in N(E) can be omitted because it simplifies in the ratio. The expressions, without this factor, are respectively:

$$N_{2D} = \int E^{1/2} e^{-E/KT} dE = (KT)^2$$
(3.5)

(non-degenerate 2D) and:

$$N_{3D} = \int E^{3/2} e^{-E/KT} dE = \frac{3\pi^{1/2}}{4} (KT)^{5/2}$$
(3.6)

(non-degenerate 3D). It has to be noticed that for the degenerate semiconductor the average is calculated by a weighting function such that:

$$\left\langle \varphi(E) \right\rangle = \frac{\int \varphi(E)EN(E) \frac{\partial f_0}{\partial E} dE}{\int EN(E) \frac{\partial f_0}{\partial E} dE}$$
(3.7)

where  $f_0$  is the Fermi-Dirac density of probability and is approximately 1 when  $E < E_F$  and 0 when  $E > E_F$ .

### 3.5 2D $\mu$ w-IR phonon and alloy scattering mobility\*

The phonon scattering is the dominant scattering mechanism contributing to the mobility of 2D carriers in semiconductors in a high temperature regime. In this paragraph it is evaluated the most general form to write the real part of the  $\mu$ w mobility for the phonon and alloy scattering in a non-degenerate semiconductor or a semiconductor where all the carriers hold an energy near to Fermi energy. This assumption implies that the spectrum of energy assumed by the carriers does not depend from the energy, so the scattering time is fixed and no average on the statistics is needed. As already seen, the real part of the mobility depends on the ratio between:

$$\operatorname{Re}\sigma_{0} = \operatorname{Re}\left[\frac{ne^{2}}{m^{*}}\frac{\tau\left(1+j\omega\tau\right)}{\left(j\omega\tau+1\right)^{2}+\left(\omega_{c}\tau\right)^{2}}\right] = \frac{ne^{2}}{m^{*}}\frac{\tau\left[1+\left(\omega_{c}^{2}+\omega^{2}\right)\tau^{2}\right]}{\left[1+\left(\omega_{c}^{2}-\omega^{2}\right)\tau^{2}\right]^{2}+4\omega^{2}\tau^{2}}$$
(3.8)

$$|\operatorname{Re}\sigma_{1}| = \operatorname{Re}\left[\frac{ne^{2}}{m^{*}}\frac{\omega_{c}\tau^{2}}{(i\cos\tau+1)^{2}+(\cos\tau)^{2}}\right] = \frac{ne^{2}}{m^{*}}\frac{\omega_{c}\tau^{2}\left[1+(\omega_{c}^{2}-\omega^{2})\tau^{2}\right]}{[1-(\omega_{c}^{2}-\omega^{2})\tau^{2}]^{2}}$$
(3.9)

$$\left|\operatorname{Re}\sigma_{1}\right| = \operatorname{Re}\left[\frac{n^{c}}{m^{*}}\frac{\omega_{c}\tau}{\left(j\omega\tau+1\right)^{2}+\left(\omega_{c}\tau\right)^{2}}\right] = \frac{n^{c}}{m^{*}}\frac{\omega_{c}\tau\left[1+\left(\omega_{c}-\omega^{2}\right)\tau\right]}{\left[1+\left(\omega_{c}^{2}-\omega^{2}\right)\tau^{2}\right]^{2}+4\omega^{2}\tau^{2}}$$
(3.9)

The explicit evaluation leads to:

$$\mu_{\rm H} = \frac{1}{\rm B} \frac{\left|{\rm Re}\,\sigma_{\rm I}\right|}{{\rm Re}\,\sigma_{\rm 0}} = \frac{\omega_c \tau \left[1 + \left(\omega_c^2 - \omega^2\right)\tau^2\right]}{B\left[1 + \left(\omega_c^2 + \omega^2\right)\tau^2\right]} \tag{3.10}$$

There are two important considerations suggested by the shape of this equation. First, it has to be noticed that when the frequency of applied field is zero, the dummy not-time-averaged d.c. case is covered. Since:

$$\mu_{H}\Big|_{\omega=0} = \mu_{H(d.c.)} \tag{3.11}$$

a frequency Hall factor can be expressed as:

$$R_{\omega} = \frac{\mu_{H}}{\mu_{H(d,c)}} = \frac{1 + (\omega_{c}^{2} - \omega^{2})\tau^{2}}{1 + (\omega_{c}^{2} + \omega^{2})\tau^{2}}$$
(3.12)

Second, as it can be seen in Figure 3.a, for every values of  $\omega_c$ , there is always a value of  $\omega$  such that the  $\mu w$  mobility vanishes.



Figure 3.a The Frequency Hall Factor for phonon and alloy scattering of a non-degenerate semiconductor as a function of the cyclotron frequency and the  $\mu$ w-IR field at unitary scattering time  $\tau$ . This function vanishes at every value of the cyclotron frequency and causes the vanishing of the  $\mu$ w-IR mobility.

This happens when:

$$\omega^2 = \tau^{-2} + \omega_c^2 \tag{3.13}$$

and holds even in the limit of low field ( $\omega_c^2 \ll \tau^{-2}$ ). This analysis has been calculated explicitly in force of the not spread values in the energy spectrum.

### 3.6 2D $\mu$ w-IR ionized impurity scattering mobility\*

Generally speaking, the impurity scattering may dominate the mobility in the low temperature range [RID88] and gives the principal contribution in mobility versus the doping carrier density plot of a bulk semiconductor. For what concerns a two-dimensional semiconductor, this is in general not the main contribution, essentially because of scatter centers that are located not in the layer plane but at a distance from it [SHI98] and primarily because of the screening of the charge: the high sheet concentration (roughly  $10^{12}$  cm<sup>-2</sup>) is also responsible for a high degree of screening effect that virtually eliminates Coulomb scattering [ALI91]. In this paragraph it will be examined an interesting two-dimensional case where the screening effect may be reduced and the impurity scattering  $\mu w$  effects appear governed by a non-degenerate statistics. In this case the low temperature dominant scattering mechanism is due to ionized impurities [KEL95, page. 116]

# 3.6.1 General expression of $\mu$ w-IR mobility for non-degenerate impurity scattering

The function of the frequency that it has to be specified is the mobility, and the interest is to find its analytical expression:

$$\mu_{H} = \frac{1}{B} \frac{\left| \operatorname{Re}\langle \sigma_{1} \rangle \right|}{\operatorname{Re}\langle \sigma_{0} \rangle} = \frac{\left\langle \frac{\omega_{c} \tau^{2}}{\left( 1 + \omega^{2} \tau^{2} \right)^{2}} \left( 1 - \omega^{2} \tau^{2} \right) \right\rangle}{B \left\langle \frac{\tau}{1 + \omega^{2} \tau^{2}} \right\rangle}$$
(3.14)

even in presence of a quite complicated average. The assumption in the following is that the semiconductor is non-degenerate. The full evaluation of the mobility in this case requires the exploitation of integrals of the form:

$$\left\langle \frac{\tau^{l}(E)}{\left(1+\omega^{2}\tau^{2}\right)^{r}}\right\rangle = \frac{\int \frac{\tau^{l}(E)}{\left(1+\omega^{2}\tau^{2}\right)^{r}} E^{p} e^{-E/KT} dE}{\int E^{p} e^{-E/KT} dE}$$
(3.15)

for r = 1,2 respectively for the denominator and the numerator in the mobility expression and l = 1,2,4, where *p* and *s* are reported for 2D and 3D cases in Table 3.II.

	2D	3D
$\tau(E)$	aE(s=-1)	$aE^{3/2}(s=-3/2)$
$EN\left( E ight)$	cE(p=1)	$cE^{3/2}(p=3/2)$

Table 3.II Scattering time and power-low factor of weight function of energy in 2D and 3D cases.

The result of the integral may be expressed in a very general form, just specifying the value of s, which depends on scattering kind. The factor c appearing in the Table 3.II is the constant factor of the DOS and it disappears in the ratio so it can be set equal to unit: c = 1. Let's now express the integrals involved in the Eq. (3.15) in the form:

$$I_{lr}(\beta_{s}) = \int \frac{\tau^{l}(E)}{(1+\omega^{2}\tau^{2})^{r}} E^{p} e^{-E/KT} dE = a^{l} \int \frac{E^{-ls+p}}{(1+\omega^{2}a^{2}E^{-2s})^{r}} e^{-E/KT} dE =$$
  
=  $(KT)^{p-ls+1} a^{l} \int \frac{x^{p+(2r-l)s}}{(x^{2s}+\beta_{s})^{r}} e^{-x} dx \equiv (KT)^{p-ls+1} a^{l} I_{lr}'(\beta_{s})$  (3.16)

where:

$$\beta_s = \omega^2 a^2 \left( KT \right)^{-2s} \tag{3.17}$$

The interest holds for the three cases where r = 1 when l = 1 and r = 2 when l = 2,4. It will be shown in the next that these integrals may be expressed in terms of the generalized hypergeometric function.

#### **3.6.2** Non degeneracy in two-dimensional semiconductors

To justify the assumption that it will be made in the following, it has to be shown that there is a condition where the two-dimensional semiconductors leave the degeneracy condition and become non-degenerate. The reference quantity is the Fermi energy and comparing it with the order of the band gap in GaAs shows that the non-degeneracy may be realized.

The case here examined is that of ultra-low density two-dimensional semiconductors (the density may go down to the value of  $10^{10}$  cm<sup>-2</sup>). Since the degeneracy is lost, the evaluation of the mobility has to be done averaging as shown in previous sections of this chapter, valid for non-degenerate semiconductors.

Following the procedure to evaluate the Fermi energy reported by Ziman for bulk 3D semiconductors [ZIM69], it is possible to estimate the Fermi energy of 2D semiconductors. In this case:

$$4\pi k_F^2 \frac{2}{4\pi^2} = n \tag{3.18}$$

so:

$$E_F = \frac{\pi \eta^2 n}{4m^*} \tag{3.19}$$

The non-degenerate case holds if  $E_F \ll kT$  [ZIM69, pag.117] and the evaluation can be done using values reported in Table 3.III. The Fermi energy results  $E_F = 1.33 \ 10^{-37} \ n(\text{m}^{-2}) \text{ J} = 1.33 \ 10^{-33} \ n(\text{cm}^{-2}) \text{ J}$ .

Quantity	Quantity Value	
k	$1.380 \ge 10^{-23}$	J/deg
$m_e$	9.981 x 10 <sup>-31</sup>	Kg
η	$1.055 \times 10^{-34}$	Js
<i>m</i> *(4K)	$0.066 m_e$	

Table 3.III Values used to evaluate the non-degeneracy condition in GaAs.

The validity of the non-degenerate statistics can be searched in some ranges of reproducible temperature and sheet density of carriers [PAS02]. Results are displayed in Table 3.IV and they show that the situation analyzed in this paragraph may be physically realized.

$E_F/kT$		kT J (TK)		
		$1.380 \ 10^{-23} \ (1)$	$1.380 \ 10^{-22} (10)$	4.41 10 <sup>-21</sup> (300)
	$10^{9}$	0.96 x 10 <sup>-1</sup>	0.96 x 10 <sup>-2</sup>	3.2 x 10 <sup>-4</sup>
$n(\text{cm}^{-2})$	$10^{10}$	$0.96 \ge 10^{\circ}$	0.96 x 10 <sup>-1</sup>	3.2 x 10 <sup>-3</sup>
	$10^{11}$	$0.96 \ge 10^1$	0.96 x 10 <sup>0</sup>	3.2 x 10 <sup>-2</sup>
	$10^{12}$	$0.96 \ge 10^2$	0.96 x 10 <sup>1</sup>	$3.2 \times 10^{-1}$

Table 3.IV Comparison between the Fermi energy and the kT energy value in joule using GaAs effective mass. The gray scale shows that non-degenerate regime appears at sufficient low density and high temperature. It has to be noticed that the Fermi energy changes from its value when the temperature is increased.

#### 3.6.3 $\mu$ w-IR Mobility expression of ultra-low density 2D semiconductors

Two-dimensional semiconductors correspond in general to a degenerate carrier gas confined in the quantum well at the interface between different gap materials such as GaAs/AlGaAs interface. Under the condition that the density is very low, the impurity scattering may become relevant [SHI98]. If the temperature is high enough and the density is low enough to let the gas to be non-degenerate, the explicit application of energy average to this interesting physical case such as the impurity scattering can be done. Ultra-low density two-dimensional carrier gases are realized and studied in the metal-insulator transition context as done by Simmons *et al.* [SIM98] which observed a metal-insulator transition in an ultra-low density two-dimensional hole gas formed in a high quality GaAs/AlGaAs heterostructure where the range of density spaces around  $1 \cdot 10^{10}$  where a relevant contribution is also due to the electron-electron interactions.

In the **2D** case s = -1 and p = 1, and it is useful to set the exponent:

$$b = (2r - l)s + p = l - 2r + 1$$
(3.20)

In the d.c. case  $\beta_s = 0$ , and the integral equals:

$$I_{lr}(0)_{2D} = (KT)^{p-ls+1} a^{l} \Gamma(l+\frac{1}{2}) = (KT)^{p-ls+1} a^{l} I_{lr}'(0)_{2D}$$
(3.21)

This is both a definition for  $I_{lr}$  and  $I'_{lr}$ . In general at  $\mu$ w-IR the integrals equal (for Re[*b*] > -3, Arg[ $\beta_s$ ]  $\neq \pi$ ):

$$I_{l1}(\beta_{s}) = (KT)^{p-ls+1} a^{l} \left\{ \beta_{s}^{-1} \Gamma(1+b)_{1} F_{2} \left[ 1, \left(\frac{1}{2} - \frac{b}{2}, -\frac{b}{2}\right), -\frac{1}{4\beta_{s}} \right] - \frac{\pi}{2} \beta_{-1}^{-(b+3)/2} \left[ \cos \sqrt{\frac{1}{\beta_{s}}} \sec \frac{b\pi}{2} + \sin \sqrt{\frac{1}{\beta_{s}}} \csc \frac{b\pi}{2} \right] \right\}$$

$$I_{l1}(\beta_{-1})_{2D} = (KT)^{l+2} a^{l} \left\{ \beta_{-1}^{-1} \Gamma(1+b)_{1} F_{2} \left[ 1, \left(\frac{1}{2} - \frac{b}{2}, -\frac{b}{2}\right), -\frac{1}{4\beta_{-1}} \right] - \frac{\pi}{2} \beta_{-1}^{-(b+3)/2} \left[ \cos \sqrt{\frac{1}{\beta_{-1}}} \sec \frac{b\pi}{2} - \sin \sqrt{\frac{1}{\beta_{-1}}} \csc \frac{b\pi}{2} \right] \right\}$$

$$(3.22a)$$

$$(3.22b)$$

and (for  $\operatorname{Re}[b] > -5$ ,  $\operatorname{Arg}[\beta_s] \neq \pi$ ):

$$I_{l2}(\beta_{s}) = (KT)^{p-ls+1} a^{l} \left\{ \beta_{s}^{-2} \Gamma(1+b)_{1} F_{2} \left[ 2, \left(\frac{1}{2} - \frac{b}{2}, -\frac{b}{2}\right), -\frac{1}{4\beta_{s}} \right] - \frac{\pi}{4} \beta_{-1}^{-(b+5)/2} \left[ \left( (3+b) \cos \sqrt{\frac{1}{\beta_{s}}} - \sqrt{\frac{1}{\beta_{s}}} \sin \sqrt{\frac{1}{\beta_{s}}} \right) \sec \frac{b\pi}{2} + \left( (3+b) \sin \sqrt{\frac{1}{\beta_{s}}} + \sqrt{\frac{1}{\beta_{s}}} \cos \sqrt{\frac{1}{\beta_{s}}} \right) \csc \frac{b\pi}{2} \right] \right\}$$

$$(3.23a)$$

$$I_{l2}(\beta_{-1})_{2D} = (KT)^{l+2} a^{l} \left\{ \beta_{-1}^{-2} \Gamma(1+b)_{1} F_{2} \left[ 2, \left(\frac{1}{2} - \frac{b}{2}, -\frac{b}{2}\right), -\frac{1}{4\beta_{-1}} \right] - \frac{\pi}{4} \beta_{-1}^{-(b+5)/2} \left[ \left( (3+b) \cos \sqrt{\frac{1}{\beta_{-1}}} - \sqrt{\frac{1}{\beta_{-1}}} \sin \sqrt{\frac{1}{\beta_{-1}}} \right) \sec \frac{b\pi}{2} + \left( (3+b) \sin \sqrt{\frac{1}{\beta_{-1}}} + \sqrt{\frac{1}{\beta_{-1}}} \cos \sqrt{\frac{1}{\beta_{-1}}} \right) \csc \frac{b\pi}{2} \right] \right]$$

$$(3.23b)$$

The integrals have been evaluated explicitly by using Wolfram Mathematica 3 software application. This analysis provides both the analytical expression of the  $\mu$ w-IR Mobility and of the Frequency Hall factor. The normalizing factors of averages simplify so in general:

$$\mu_{H} = \frac{1}{B} \frac{\left| \operatorname{Re} \langle \sigma_{1} \rangle \right|}{\operatorname{Re} \langle \sigma_{0} \rangle} = \frac{\omega_{c} \left( I_{22} \left( \beta_{s} \right) - \omega^{2} I_{42} \left( \beta_{s} \right) \right)}{B I_{11} \left( \beta_{s} \right)} = \frac{a K T \omega_{c} \left( I_{22}^{\prime} \left( \beta_{s} \right) - \beta_{s} I_{42}^{\prime} \left( \beta_{s} \right) \right)}{B I_{11}^{\prime} \left( \beta_{s} \right)}$$
(3.24)

and for ionized impurity scattering you have:

$$\mu_{H} = \frac{1}{B} \frac{\left| \operatorname{Re} \langle \sigma_{1} \rangle \right|}{\operatorname{Re} \langle \sigma_{0} \rangle} = \frac{a K T \omega_{c} \left( I_{22}^{\prime} (\beta_{-1}) - a^{2} (K T)^{2} \omega^{2} I_{42}^{\prime} (\beta_{-1}) \right)}{B I_{11}^{\prime} (\beta_{-1})}$$
(3.25)

The Frequency Hall factor results:

$$R_{\omega} = \frac{\mu_{H}}{\mu_{H(d.c.)}} = \frac{\left(I_{22}(\beta_{-1}) - \omega^{2}I_{42}(\beta_{-1})\right)}{I_{11}(\beta_{-1})} \frac{I_{11}(0)}{I_{22}(0)} = \frac{\left(I_{22}'(\beta_{-1}) - a^{2}(KT)^{2}\omega^{2}I_{42}'(\beta_{-1})\right)}{I_{11}'(\beta_{-1})} \frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{5}{2})}$$
(3.26)

This gives a quantitative evaluation of the  $\mu$ w-IR effects caused by scattering impurities.

# 4 Transport and supersymmetry in disordered systems

There is a totally different approach developed by Konstantin Efetov after the first application of supersymmetry in condensed matter physics in a paper of Parisi and Sourlas [PAR79], which contains deep connections with the perturbative one and it is based on a different formalism. The main idea comes from usual techniques developed in quantum and statistical field theory [ZIN89] where, at the transition point, universal properties are not determined by the function governing microscopic interactions by the smallest constituent of the system. This finds an application by identifying the carriers running in a random distribution of impurities with a general interactive theory at the phase transition (it does not matter the kind of interaction) where Goldstone modes of the breaking symmetry are diffusion modes of the previous picture (Par. 1). The choice of the model falls onto the supersymmetric  $\sigma$ -model and the universality class giving physical results is d = 0. Notice that the choice of a particular model is not relevant for the final result so the choose one is simply the most easy to performs the calculations. This picture describes localization, mesoscopics, quantum chaos, integer quantum Hall effect. This suggests that supersymmetry reflects some hidden symmetries in disordered and chaotic systems. This chapter delineates essentials of this powerful approach and evaluates explicitly IR corrections to the conductivity.

### 4.1 Supersymmetry in disordered systems

In this paragraph are reported essentials of the supersymmetric  $\sigma$ -model and the application to IR conductivity.

#### 4.1.1 Non-linear supermatrix $\sigma$ -model

Supersymmetric theories have been developed for particle physics following the idea that it may be a symmetry that interrelates bosons and fermions, in order to solve in a natural way the hierarchy problem of the mass of the light Higgs boson [COL89]. They are based on the use of anticommuting variables extending a regular theory expressed in terms of commuting variables. Note that, contrary to the particle physics use, in condensed matter there is not an immediate physical meaning to attribute to anticommuting fields, and the use owns a sense because the system is considered in a critical condition with respect to a breaking hidden symmetry. Thanks to the properties of the integration in the superspace, the random potential included in Lagrangian can be averaged before

than making explicit calculations and the consequence is a manageable theory to perform perturbative or analytical calculations. The Lagrangian corresponding to Hamiltonian (1.21) after the average on random potential is a QFT of expression:

$$L = \int \left[ -i\overline{\psi} \left( \varepsilon \left( -i\nabla_r \right) - \varepsilon + \frac{\omega}{2} \right) \psi + \frac{1}{4\pi\nu\tau} \overline{\psi} \psi - \frac{i(\omega + i\delta)}{2} \overline{\psi} \Lambda \psi \right] d^d r$$
(4.1)

where  $\psi$  are 8 components supervectors, v and  $\tau$  come from random potential definition (1.22) and  $\Lambda$  is the diagonal supermatrix

$$\Lambda = \begin{pmatrix} I_{4x4} & 0\\ 0 & -I_{4x4} \end{pmatrix} \tag{4.2}$$

The  $i\delta$  term in used to remove poles in propagators along the real axis and perform the integral over it. By using a Hubbard-Stratonovich transformation this model can be reduced to a very simpler one, well-known in statistical field theory, i.e. the  $\sigma$ -model in the supersymmetric form. After obtaining the supermatrix Q, implicitly expressed by this integral equation:

$$Q = \frac{i}{\pi} \int_{-\infty}^{+\infty} d\xi \left( \xi + \frac{1}{2} (\omega + i\delta) \Lambda + \frac{iQ}{2\tau} \right)^{-1}$$
(4.3)

it can be found the free energy functional of the model:

$$F[Q] = \frac{\pi v}{8} \operatorname{str} \int d^{d} r \left( D_{0} (\nabla Q)^{2} + 2i(\omega + i\delta) \Lambda Q \right)$$
(4.4)

where  $D_0$  is the classical diffusion coefficient, with constraint:

$$Q = V\Lambda \overline{V}, V\overline{V} = I_{8x8} \tag{4.5}$$

where V is an arbitrary unitary supermatrix [EFE82a, EFE82b]. This is the new starting point to let physics be successfully described. This model is similar to the Heisemberg model for ferromagnets. The frequency plays a role of an external field: at  $\omega = 0$  the symmetry is realized. When it assumes non-zero values the symmetry of the Lagrangian is broken and Goldstone modes appear; they can be identified with diffusion modes of the perturbative approach.

#### 4.1.2 IR conductivity correction by using supersymmetry

Performing explicit calculations to obtain conductivity in the high frequency limit, where deviations of the Q matrix from  $\Lambda$  are small, this picture leads to recover a perturbative result, which can be found by using the diffusion modes. This connection confirms that the supersymmetric approach leads to correct answers, comparable with the known ones, and it can be used as a powerful tool in non-perturbative calculations.

In the IR limit  $\omega \to \infty$  specified, it is found that they both give:

$$\sigma(\omega) = \sigma(0) \left( 1 - \frac{1}{\pi \nu} \int \frac{d^d k}{(2\pi)^d} \frac{1}{D_0 \overline{k}^2 - i\omega} \right)$$
(4.6)

where v appears as an external field, and  $D_0$  is the classical diffusion coefficient. This integral does not converge at most interesting dimensionalities, but finiteness is guaranteed by physical cutoffs on momenta. This particular result can be obtained by using perturbative approach also, but this treatment allows more applications and shows that universal properties cover disordered and chaotic systems revealing an hidden symmetry of nature.

### 4.2 IR conductivity at physical dimensionality\*

Here are explicitly evaluated the IR corrections at generic and physical dimensionalities. In order to evaluate impurity effects in the high frequency limit, an explicit evaluation of IR conductivity can be done at a generic dimensionality:

$$\sigma(\omega) = \sigma(0) \left( 1 - \frac{1}{\pi \nu} \int \frac{d^{d}k}{(2\pi)^{d}} \frac{1}{D_{0}\bar{k}^{2} - i\omega} \right) =$$

$$= \sigma(0) \left( 1 - \frac{1}{\pi \nu D_{0}} \frac{2\pi^{d/2}}{(2\pi)^{d} \Gamma(\frac{d}{2})} \int_{0}^{+\infty} dk \frac{k^{d-1}}{k^{2} - i\omega/D_{0}} \right) =$$

$$= \sigma(0) \left[ 1 - \frac{1}{2^{d-1} \pi^{d/2+1} \Gamma(\frac{d}{2}) D_{0} \nu} \int_{0}^{+\infty} dk \frac{k^{d+1}}{k^{4} + \omega^{2}/D_{0}^{2}} \right] -$$

$$- i\sigma(0) \left[ \frac{\omega}{2^{d-2} \pi^{d/2} \Gamma(\frac{d}{2}) D_{0}^{3}} \int_{0}^{+\infty} dk \frac{k^{d-1}}{k^{4} + \omega^{2}/D_{0}^{2}} \right] =$$

$$= \operatorname{Re} \sigma(\omega) + i \operatorname{Im} \sigma(\omega)$$

$$(4.7)$$

where  $\Gamma$  represents the Gamma function. The reduction of the integral to a radial integration along just one coordinate requires the factor representing the hypervolume of a *d*-dimensional sphere in the momenta space.

This analysis is interested in the real part of the conductivity because it relates to the mobility, perturbing the d.c. one. One can evaluate the correction term by integrating at the interesting dimensionality, if necessary using a physical cutoff on momenta when integral diverges. The results obtained by integrating show the same functional dependence on the cut-off momentum K of that reported by Lee and Ramakrishan [LEE85].

#### **1D IR conductivity correction**

In this case, valid for quantum wires (1D), the integration does not require cutoffs.

$$\int_{0}^{+\infty} dk \frac{k^{d+1}}{k^{4} + \omega^{2} / D_{0}^{2}} \bigg|_{d=1} = \sqrt{\frac{D_{0}}{\omega}} \frac{\pi}{2\sqrt{2}}, \operatorname{Arg}[\omega^{2} / D_{0}^{2}] \neq \pi$$
(4.8)

so:

$$\operatorname{Re}[\sigma(\omega)|_{d=1}] = \sigma(0) \left( 1 - \frac{1}{\pi \nu D_0} \frac{2\pi^{1/2}}{(2\pi)\Gamma(\frac{1}{2})} \sqrt{\frac{D_0}{\omega}} \frac{\pi}{2\sqrt{2}} \right) = \sigma(0) \left( 1 - \frac{1}{\sqrt{2D_0\omega^3}} \right)$$
(4.9)

#### **2D IR conductivity correction**

In this case the integral diverges at high momentum, so it can be considered a physical range for momentum k:

$$0 < k < \frac{1}{\lambda} = K \tag{4.10}$$

where the minimum physical length is  $\lambda$ , i.e. the mean free path [RID95].  $\lambda$  is of the order of tens of nanometers in 2D degenerate semiconductors.

$$\int_{0}^{K} dk \frac{k^{d+1}}{k^{4} + \omega^{2} / D_{0}^{2}} \bigg|_{d=2} = \frac{1}{4} \ln \frac{\omega^{2} / D_{0}^{2} + K^{2}}{\omega^{2} / D_{0}^{2}}$$
(4.11)

so:

$$\operatorname{Re}[\sigma(\omega)|_{d=2}] = \sigma(0) \left( 1 - \frac{1}{\pi \nu D_0} \frac{2\pi}{(2\pi)^2 \Gamma(1)} \frac{1}{4} \ln \frac{\omega^2 / D_0^2 + K^2}{\omega^2 / D_0^2} \right)$$
  
=  $\sigma(0) \left( 1 - \frac{1}{4\pi D_0 \omega} \ln \frac{\omega^2 / D_0^2 + K^2}{\omega^2 / D_0^2} \right)$  (4.12)

#### **3D IR conductivity correction**

In this case valid for bulk semiconductors (3D) the integral again diverges and it can be used the same cutoff used in section 1.1.4.b. It is more complicated and gives:

$$F(\omega, K) \equiv \int_{0}^{+\infty} dk \frac{k^{d+1}}{k^{4} + \omega^{2} / D_{0}^{2}} \bigg|_{d=3}$$

$$= K + \frac{1}{4} \sqrt{\frac{2\omega}{D_{0}}} \bigg[ \tan^{-1} \bigg( 1 - \sqrt{\frac{2D_{0}}{\omega}} K \bigg) - \tan^{-1} \bigg( 1 + \sqrt{\frac{2D_{0}}{\omega}} K \bigg) \bigg] + \frac{1}{8} \sqrt{\frac{2\omega}{D_{0}}} \ln \frac{\frac{\omega}{D_{0}} - \sqrt{\frac{2\omega}{D_{0}}} K + K^{2}}{\frac{\omega}{D_{0}} + \sqrt{\frac{2\omega}{D_{0}}} K + K^{2}}$$
(4.13)

so:

$$\operatorname{Re}[\sigma(\omega)|_{d=3}] = \sigma(0) \left( 1 - \frac{1}{\pi \nu D_0} \frac{2\pi^{3/2}}{(2\pi)^3 \Gamma(\frac{3}{2})} F(\omega, K) \right)$$
(4.14)

In this case, substituting actual values in Eq. (4.14), the contribution may be not irrelevant at microwave frequency. In effect for GaAs one can consider  $D_0=2 \ 10^{-4} \text{m}^2/\text{s}$  and  $1/\lambda_d = \text{K} = 5 \ 10^8 \text{m}^{-1}$ , since  $\tau$  is of the order of  $10^{-13}$ s and  $\omega > \tau^{-1}$ , the correction is of the order of percents around 1000 GHz, at the limit of validity of the scheme.

# **APPENDIX A – Relativistic Density of States** in *d*-dimensional Electron Gas\*

This Appendix extends the result obtained for the non-relativistic case (Paragraph 1.2). Symbols and letters follow the same notation of that paragraph.

#### **Evaluation of the DOS**

Following the same scheme of the non-relativistic case, it is necessary to consider the analytical continuation at d dimension to express the number of possible states. It can be considered (1.8) so that:

$$dn = \prod_{i}^{d} dn_{i} = \left(\frac{h}{2L}\right)^{-d} d^{d} p = \frac{2\pi^{d/2}}{2^{d} \Gamma(\frac{d}{2})} \left(\frac{h}{2L}\right)^{-d} p^{d-1} dp$$
(A.0)

The relationship between energy and momentum is described by the relativistic expression:

$$p = \sqrt{\frac{E^2}{c^2} - m^2 c^2}, \quad dp = \frac{E/c}{\sqrt{(E/c)^2 - m^2 c^2}} d(E/c)$$
(A.1)

The substitution gives:

$$dn = g(E)dE = \frac{2\pi^{\frac{d}{2}}}{2^{d} \Gamma(\frac{d}{2})} \left(\frac{h}{2L}\right)^{-d} \left((E/c)^{2} - m^{2}c^{2}\right)^{\frac{d-2}{2}} (E/c)d(E/c)$$
(A.2)

Including spin degeneracy for particles with spin s:

$$g(E) = (2s+1)\frac{2\pi^{\frac{d}{2}}}{2^{d}\Gamma(\frac{d}{2})} \left(\frac{2L}{h}\right)^{d} \left((E/c)^{2} - m^{2}c^{2}\right)^{\frac{d-2}{2}} (E/c)d(E/c)$$
(A.3)

Note that the minimum energy value is  $m^2c^2$ . From a functional point of view, the energy power law in the vicinity of the lowest possible value is the same than that found for the non-relativistic case.

# **APPENDIX B – Complex Expression Linking the Mobility and the Dielectric Constant**

In this Appendix it is obtained the equation linking the mobility with the dielectric constant in the complex domain used in Paragraphs 2 for homogeneous media.

When expressed in absence of a magnetic field, the mobility tensor relates to the conductivity linearly by the expression of its diagonal elements:

$$\sigma(\omega) = ne \ \mu(\omega) \tag{D.1}$$

By considering both the frequency and the mobility as complex valued, it holds:

$$\varepsilon(\omega) = \varepsilon'(\omega) + j \frac{4\pi \ \sigma(\omega)}{\omega}$$
  
=  $\varepsilon'(\omega) + j \frac{4\pi \ ne \ \mu(\omega)}{\omega}$  (D.2)  
=  $\left(\varepsilon'(\omega) - \frac{4\pi \ ne \ [\mu''(\omega)\omega' - \mu'(\omega)\omega'']}{|\omega|^2}\right) + j \frac{4\pi \ ne \ [\mu'(\omega)\omega' + \mu''(\omega)\omega'']}{|\omega|^2}$ 

For the purposes of this analysis it is sufficient to consider the real part of mobility, since under the condition that the imaginary part of the (angular) frequency is small with respect to the real part:

$$\omega'' << \omega' \tag{D.3}$$

the Eq. (D.2) reduces to:

$$\varepsilon(\omega) = \left(\varepsilon'(\omega) - \frac{4\pi ne\left[\mu''(\omega)\omega' - \mu'(\omega)\omega''\right]}{|\omega|^2}\right) + j\frac{4\pi ne \mu'(\omega)\omega'}{|\omega|^2}$$
(D.4)

without any hypothesis about the real and imaginary part of the mobility. This gives:

$$\varepsilon''(\omega) = \frac{4\pi ne \,\mu'(\omega)\omega'}{|\omega|^2} \tag{D.5}$$

for materials with low losses.

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