## The Einstein Relation In Quantum Wires Of Heavily Doped Nonlinear Optical And Optoelectronic Materials: Simplified Theory And Suggestion For Experimental Determination

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#### Abstract

We study the Einstein relation for the diffusivity- mobility ratio (DMR) in quantum wires (QW) of heavily doped non-linear materials on the basis of a newly formulated electron dispersion law considering all types of anisotropies and the influence of crystal field splitting. The quantum confined optoelectronic III-V compounds form a special case of our generalized analysis. It has been found that the DMR increases with increasing electron concentration per unit length in oscillatory manners and the nature of oscillations are totally band structure dependent. An experimental method of determining the DMR in nanostructures having arbitrary dispersion law has been suggested

### INTRODUCTION

It is well known that the DMR occupies a central position in the whole field of nanoscience and technology since the diffusion constant (a quantity very useful for device analysis whose exact experimental determination is rather difficult) is derived from this ratio by knowing the experimental values of the mobility. In addition, it is more accurate than any of the individual relations for the diffusivity or the mobility, which is two widely used quantities of carrier transport of nanodevices. Landsberg first demonstrated that the DMR under the condition of degeneracy depends only on the band structure [1]. Further more in recent years, the connection of the DMR with the velocity autocorrelation function, its relation with the noise power and the formulations of the DMR in various nanostructures have extensively been investigated [1-3]. Nevertheless, it appears from the literature that the DMR in OWs of heavily doped nonlinear optical and optoelectronic materials has yet to be investigated in details by considering all types of anisotropies using the framework of Gaussian band tails as formed in heavily doped materials. In this context it is noted that Kildal [4] proposed the energy spectrum of the conduction electrons in non-linear optical materials under the assumptions of isotropic momentum matrix element and isotropic spin orbit splitting respectively, although the anisotropies of the aforementioned band parameters are the significant physical features of the said compound. Besides, the III-V optoelectronic compounds finds extensive application in

distributed feedback lasers and infrared photodetectors. In what follows, we shall study the DMR in QWs of heavily doped CdGeAs<sub>2</sub>,  $Hg_{1-x}Cd_xTe$  and  $In_{1-x}Ga_xAs_yP_{1-y}$  lattice matched to InP on the basis of a newly formulated electron dispersion law by considering the aforementioned anisotropies of the energy bands constants together with the inclusion of crystal field splitting constant respectively. We shall also suggest an experimental method of determining the DMR in nanostructures having arbitrary dispersion laws.

#### THEORETICAL BACKGROUND

The dispersion relation of the conduction electrons in bulk specimens of non-linear optical materials within the framework of **k.p** formalism can be expressed as [5]

$$\gamma(E) = f_1(E)k_x^2 + f_2(E)k_z^2$$
(1)

where the notations are defined in the above reference.

The Gaussian distribution of F(V) of the impurity potential is given by

$$F(V) = \left(\pi \eta^2\right)^{-1/2} \exp\left(-V^2/\eta^2\right)$$
(2)

where  $\eta$  is the impurity screening potential.

Combining Equations. (1) and (2), the dispersion relation of the conduction electrons in heavily doped non-linear optical material can be written, after tedious mathematics, as

$$\frac{k_z^2}{Q_1(E,\eta)} + \frac{k_z^2}{Q_2(E,\eta)} = 1$$
(3)

$$Q_{1}(E,\eta) = \frac{2m_{\parallel}^{*}}{\hbar^{2}} \left[ X(E,\eta) + iY(E,\eta) \right],$$

$$Q_{2}(E,\eta) = \frac{2m_{\perp}^{*}}{\hbar^{2}} \left[ \frac{X(E,\eta) + iY(E,\eta)}{\left(\frac{b_{\parallel}}{b_{\perp}}\frac{c_{\parallel}}{c_{\perp}}\right) + V(E,\eta) + iW(E,\eta)} \right]$$

and the other notations are functions of E and  $\eta$ . The electron concentration per unit length in QWs of heavily doped non-linear optical materials can be written as

$$n_0 = \frac{2}{\pi} C_2 [T_1 + T_2]$$
(4)

here 
$$C_2 = \sum_{n_z=1}^{n_{zmax}} \sum_{n_y=1}^{n_{ymax}}$$
,  $T_1 = \text{Real part of } \left[ Q_1(E',\eta) \left\{ 1 - \frac{(n_x \pi/d_x)^2 + (n_z \pi/d_z)^2}{Q_2(E',\eta)} \right\} \right]^{1/2}$ 

 $E' = E_F + i\Gamma$ ,  $E_F$  is the Fermi energy in the present case,  $\Gamma$  is the broadening parameter,  $T_2 = \sum_{r=1}^{s} Z_r T_1$ ,  $Z_r = 2(k_B T)^{2r} (1 - 2^{1-2r}) \xi(2r) \frac{\partial^{2r}}{\partial E_F^{2r}}$ ,  $k_B$  is Boltzmann constant, T is temperature and

 $\xi(2r)$  is the Zeta function of order 2r. The DMR can, in general, be expressed as

$$D / \mu = \left(\frac{n_0}{e}\right) \left(\frac{\partial n_0}{\partial E_F}\right)^{-1}$$
(5)

Thus using equations (4) and (5) we can get the expression of DMR.

# Suggestion For Experimental Determination Of The DMR For Materials Having Arbitrary Dispersion Laws

It is well known that in the presence of a classically large magnetic field, the densityof-state function remains unchanged and the thermoelectric power is independent of scattering mechanisms. The magnitude of the thermoelectric power  $(T_0)$  in the present case can be written as [6]

$$T_0 = \left(\frac{1}{eTn_0}\right)_{-\infty}^{\infty} (E - E_F) R(E) \left[-\frac{\partial f}{\partial E}\right] dE$$
(7)

where R(E) is the total number of states and f is the distribution function. The Equation (7) can be written as

$$T_0 = \left(\pi^2 K_B^2 T / 3en_0 \right) \left(\frac{\partial n_0}{\partial E_F}\right)$$
(8)

Thus using Equations.(5) and (8) we get

$$D/\mu = \frac{\pi^2 k_B^2 T}{3e^2 T_0}$$
(9)

Thus we can experimentally determine the values of the DMR by knowing the experimental value of  $T_0$  which is a measurable quantity.

#### **RESULTS AND DISCUSSION**

Using the appropriate equations together with the parameters as given in [5] we have plotted the normalized DMR in QWs of heavily doped CdGeAs<sub>2</sub> versus electron concentration per unit length as shown in graph (a) of Fig. 1 in accordance with our generalized analysis in which the curve (b) exhibits the same dependence for  $\delta = 0$  so that we can assess the influence of crystal field splitting on the DMR for the present case. The plots (d) and (e) exhibits the same dependence for heavily doped  $Hg_{1-x}Cd_xTe$  and  $In_{1-x}Ga_xAs_vP_{1-v}$  lattice matched to InP respectively. The curve (c) has been drawn in the absence of heavy doping where as the circular plots has been obtained by using the appropriate equations together with the experimental results of  $T_0$  versus  $n_0$  as given in [7]. It appears from Fig. 1 that the DMR oscillates with  $n_0$  in different ways, which are characteristic features of dimension reduction. The oscillatory dependence is influenced by the crossing of the Fermi level by the sized quantized levels in steps. The DMR in QWs of heavily doped materials can be several orders of magnitude larger than the bulk specimens of same materials, which is also the direct consequence of electron dispersion law and the dimension reduction. For a constant temperature, the DMR varies inversely with T<sub>0</sub>. Only the experimental values of T<sub>0</sub> for any material as a function of electron concentration generate the experimental value of the DMR for that range of  $n_0$ . Because the experimental values of  $T_0$  in the present case excluding Hg<sub>1</sub>.  $_{\rm x}$ Cd<sub>x</sub>Te, are not available in the literature to the best of our knowledge, the theoretical formulation cannot be compared with the proposed experiment for the other types of nanostructures as considered here. Because  $T_0$  decreases with  $n_0$  in an oscillatory way, we can conclude from Equation. (9) that the DMR increases with increasing  $n_0$  in an oscillatory manner, which is also evident from Fig. 1. This statement is the indirect test of our theoretical analysis.



Fig. 1. Plot of the normalized DMR at 4.2K as a function of the electron concentration per unit length in QWs of heavily doped (a) CdGeAs<sub>2</sub> (b)  $\delta = 0$  (c) in the absence of heavy doping (d) Hg<sub>1-x</sub>Cd<sub>x</sub>Te and (e) In<sub>1-x</sub>Ga<sub>x</sub>As<sub>y</sub>P<sub>1-y</sub> lattice matched to InP respectively. The circular plots have been obtained by using Equation. (9) together with the experimental results of T<sub>0</sub> versus n<sub>0</sub> as given in [13].

Finally, it may be noted that the basic scheme of the present paper is not only to study the DMR but also to formulate the electron concentration, because the investigations of the different transport properties in nanostructures are based on the temperature dependent electron statistics in such materials with various dispersion laws.

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