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Influence of magnetic quantization on the Einstein relation in non-linear optical, optoelectronic and related materials: Simplified theory, relative comparison and suggestion for experimental determination

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Abstract

In this paper, we have investigated the Einstein relation for the diffusivity-to-mobility ratio (DMR) under magnetic quantization in non-linear optical materials on the basis of a newly formulated electron dispersion law by considering the crystal field constant, the anisotropies of the momentum-matrix element and the spin–orbit splitting constant, respectively, within the frame work of $\mathbf{k}\cdot\mathbf{p}$ formalism. The corresponding result for the three-band model of Kane (the conduction electrons of III–V, ternary and quaternary compounds obey this model) forms a special case of our generalized analysis. The DMR under magnetic quantization has also been investigated for II–VI (on the basis of Hopfield model), bismuth (using the models of McClure and Choi, Cohen, Lax and parabolic ellipsoidal, respectively), and stressed materials (on the basis of model of Seiler et al.) by formulating the respective electron statistics under magnetic quantization incorporating the respective energy band constants. It has been found, taking n-$CdGeAs_2$, n-$Hg_{1-x}Cd_xTe$, p-CdS, and stressed n-InSb as examples of the aforementioned compounds, that the DMR exhibits oscillatory dependence with the inverse quantizing magnetic field due to Subhnikov de Haas (SdH) effect with different numerical values. The DMR also increases with increasing carrier degeneracy and the nature of oscillations are totally dependent on their respective band structures in various cases. The classical expression of the DMR has been obtained as a special case from the results of all the materials as considered here under certain limiting conditions, and this compatibility is the indirect test of our generalized formalism. In addition, we have suggested an experimental method of determining the DMR for degenerate materials under magnetic quantization having arbitrary dispersion laws. The three applications of our results in the presence of magneto-transport have further been suggested.

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Keywords: Magnetic quantization; Non-linear; III–V; Experimental determination

1. Introduction

In recent years, there has been considerable interest in studying the various physical features of non-linear optical, optoelectronic and related materials because of their importance in materials science. The band structure has been observed to influence many of the electronic properties resulting in special features in these compounds. It is well known that the performance of the semiconductor devices at the device terminals and the speed of operation of modern switching devices are influenced by the degenerate carrier concentration present in these devices [1]. The simplest way of analyzing such devices is to use the Einstein relation to express the performance at the device terminal and the switching speed in terms of the carrier

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concentration [2]. Furthermore, the Einstein relation for the diffusivity-to-mobility ratio (DMR) is known to be very useful, since by being a thermodynamic relation, independent of any scattering mechanism, it is more accurate than any of the individual relations for the diffusivity or the mobility, which are considered to be the two most widely used quantities of carrier transport in semiconductors. In recent years, the connection of the Einstein relation with the velocity autocorrelation function [3], the modification due to non-linear charge transport [4] and the various formulations [5,6] of the DMR under different physical conditions have extensively been studied. This relation is useful for semiconductor homostructures [7,8], semiconductor–semiconductor heterostructures [9,10], metals–semiconductor heterostructures [11–19] and insulator–semiconductor heterostructures [20–23]. Keeping this in view, in this paper, an attempt is made to investigate the DMR under quantizing magnetic field in non-linear optical, III–V, ternaries, quaternaries, II–VI, bismuth and stressed materials on the basis of their respective carrier energy spectra. We have also suggested an experimental method of the determination of the DMR under strong magnetic quantization in this context. It is well known that the band structure of compound semiconductors can be dramatically changed by applying the external fields [24]. The effects of the quantizing magnetic field on the band structure of compound semiconductors are more striking and can be observed easily in experiments. Under magnetic quantization, the motion of the electron parallel to the magnetic field remains unaltered, while the area of the wave-vector space perpendicular to the direction of the magnetic field gets quantized in accordance with the Landau rule of area quantization in the wave-vector space [24]. The energy levels of the carriers in a magnetic field are termed as Landau levels and the quantized energies are known as Landau sub-bands. A number of interesting transport phenomena originate from the change in the basic band structure of the semiconductor in the presence of quantizing magnetic field, and these have been widely investigated and also served as diagnostic tools for characterizing the different materials having various band structures. The discreteness in the Landau levels leads to a whole crop of magneto-oscillatory phenomena, important among which are (i) Shubnikov-de Haas (SdH) oscillations in magneto-resistance; (ii) de Haas-Van Alphen oscillations in magnetic susceptibility; (iii) magneto-phonon oscillations in thermo-electric power, etc.

The non-linear optical materials are being increasingly used in light-emitting diodes, Hall pickups and thermal detectors [25–28]. Rowe and Shay [29] demonstrated that the quasi-cubic model [30] can be used to explain the observed splitting and symmetry properties of the conduction and valence bands at the zone center of the **k** space of the aforementioned compounds. The s-like conduction band is singly degenerated and the p-like valence bands are triply degenerated. The latter splits into three sub-bands due to spin–orbit and crystal field interactions. The large contribution of the crystal field splitting occurs from the non-cubic potential [31]. The experimental data on the absorption constants [32], the effective mass [33] and the optical third-order susceptibility [34] have produced strong evidence that the conduction band in the same compound corresponds to a single ellipsoid of revolution at the zone center in **k** space. Incorporating the crystal potential to the Hamiltonian, Bodnar [35] proposed a dispersion relation for the conduction electrons in the same compound by using the assumption of an isotropic spin–orbit splitting constant although the anisotropies of the band constants are important physical features of non-linear optical materials.

In Section 2.1, we have studied the magneto-DMR in non-linear optical material by formulating the generalized dispersion relation of the conduction electrons, considering the anisotropies of the effective electron masses and the spin–orbit splitting parameters together with the proper inclusion of crystal field splitting constant in the Hamiltonian within the framework of $\mathbf{k}\cdot\mathbf{p}$ formalism, which are important physical characteristics of such materials. In Section 2.2, it has been shown that the corresponding results for the magneto DMR of III–V, ternary and quaternary materials form special cases of our generalized analysis as derived in Section 2.1.

The II–VI compounds find extensive applications in infrared detectors [36], ultra high-speed bipolar transistors [37], optic fiber communications [38] and advanced microwave devices [39]. These compounds possess the appropriate direct band gap to produce light-emitting diodes and lasers from blue to red wavelengths. The Hopfield model describes the dispersion relation of both the carriers of II–VI materials, where the splitting of the two-spin states by the spin–orbit coupling and the crystalline field has been taken into account [40]. In Section 2.3, we shall study the magneto-DMR for II–VI compounds on the basis of the Hopfield model by formulating the appropriate carrier statistics and taking p-CdS as an example.

It is well-known that the carrier energy spectra in Bismuth differ considerably from simple spherical surfaces of the degenerate electron gas, and several models have been developed to describe the energy band structure of Bi. Earlier works [41,42] demonstrated that the ellipsoidal parabolic model or the one-band model could describe the carrier properties of Bi. Shoenberg [41] indicated that the de Haas-Van Alphen and cyclotron resonance experiments supported the one-band model, although the later work showed that Bi could be described by the two-band non-parabolic ellipsoidal Lax model, since the magnetic field dependence of many physical parameters of Bi supports the above model [43]. The magneto-optical results [44] and the ultrasonic quantum oscillation data [45] favor the Lax ellipsoidal non-parabolic model [46], whereas Kao [46], Dinger and Lawson [47] and Koch and Jensen [48] indicated that the Cohen model [49] is in better agreement