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The Einstein relation in quantum wells and quantum well wires: simplified theory and a suggestion for experimental determination

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Abstract
An attempt is made to study the Einstein relation for the diffusivity–mobility ratio (DMR) in quantum wells (QWs) and quantum well wires (QWWs) of tetragonal compounds on the basis of a newly formulated electron energy spectrum taking into account the combined influences of the anisotropies in the effective electron mass, the spin–orbit splitting and the presence of crystal field splitting. The corresponding results for QWs and QWWs of III–V compounds form a special case of our generalized analysis. The DMR has also been studied for QWs and QWWs of II–VI and IV–VI materials. It has been found, taking QWs and QWWs of $CdGeAs_2$, InAs, CdS and PbSe as examples, that the DMR increases with increasing carrier degeneracy and decreasing film thickness in various oscillatory manners, emphasizing the influence of dimensional quantization and the energy band constants in different cases. An experimental method for determining the DMR in QWs and QWWs having arbitrary dispersion laws has also been suggested and the present simplified analysis is in agreement with the suggested relationship. The well-known results for QWs and QWWs of relatively wide gap materials having parabolic energy bands have also been obtained as special cases from this generalized analysis under certain limiting conditions.

1. Introduction

With the advent of fine lithographic methods, molecular beam epitaxy, organometallic vapour phase epitaxy and other experimental techniques, low dimensional structures having quantum confinement in one, two and three dimensions such as quantum wells (QWs), quantum well wires (QWWs) and quantum dots have in the last few years attracted much attention not only because of their potential for uncovering new phenomena in nanotechnology, but also because of their interesting device applications [1]. In QWs, the restriction of the motion of the carriers in the direction normal to the film leads to the quantum size effect allowing two-dimensional (2D) carrier transport parallel to the surface of the film. Heterostructures based on various materials are currently being studied because of the enhancement of carrier mobility [2] and such 2D systems find extensive applications in quantum well lasers, field effect transistors, high speed digital networks, optical modulators and also in other quantum effect devices [3]. In QWWs, the carriers are quantized in two transverse directions and only one-dimensional motion of the carrier is allowed. Quantum devices such as QWW waveguides [4] and QWW transistors [5] have also been fabricated. The transport properties of electrons in QWWs may be studied by utilizing the similarities with optical and microwave waveguides. Although a considerable amount of work has been done, it appears from the recent literature that the diffusivity–mobility ratios in QWs and QWWs of tetragonal, III–V, II–VI and IV–VI materials have yet to be theoretically worked out by considering the various significant features of

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the respective energy band spectra within the framework of $\mathbf{k} \cdot \mathbf{p}$ formalism.

The diffusivity–mobility ratio (DMR) is an important relation since the diffusion constant (a quantity very useful for device analysis but whose exact experimental determination is rather difficult) can be derived from this ratio if one knows 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 are two widely used quantities in carrier transport of nanodevices. The classical value of the DMR is equal to k_BT/e (k_B, T and e are the Boltzmann constant, the temperature and the magnitude of the carrier charge respectively). This relation is the well-known Einstein relation [6]. In this conventional form it appears that the DMR increases linearly with T and is independent of electron concentration. This relation is valid for both electrons and holes. Also, the relation holds only under the condition of carrier non-degeneracy, although its validity has been suggested erroneously for degenerate materials [7]. It is well known that the performance of the electron devices at the device terminals and the speed of operation of modern switching transistors are significantly influenced by the degree of carrier degeneracy present in these devices [8]. The simplest way of analysing such devices taking into account the degeneracy of the bands is to use the appropriate Einstein relation to express the performance at the device terminals and the switching speed in terms of the carrier concentration [9]. In this context, we wish to note that the connection of the DMR with the velocity autocorrelation function and its relation with the screening length [10] and the noise power (under non-degenerate conditions) [11] have also been studied.

It is well known from the fundamental works of Landsberg [12] that the Einstein relation in degenerate materials is essentially determined by the energy band structures. It has, therefore, different values in different materials and varies with electron concentration, with the magnitude of the reciprocal quantizing magnetic field under magnetic quantization, with the quantizing electric field as in inversion layers and with the superlattice period as in quantum confined superlattices of small gap semiconductors with graded interfaces having various carrier energy spectra. The nature of these variations has been investigated by Ghatak and co-workers [13–17] and a few others [18–20]. Some of the significant features which have emerged from these studies are:

(a) the ratio increases monotonically with electron concentration in bulk semiconductors;
(b) the nature of the variations is significantly affected by the band non-parabolicity;
(c) the ratio increases with the magnitude of the quantizing electric field in inversion layers;
(d) the ratio oscillates with the inverse quantizing magnetic field under magnetic quantization due to the SdH effect;
(e) the ratio exhibits composite oscillations with the superlattice period in various types superlattices having different dispersion relations.

The above characteristics are considered as theoretical predictions and no experimental results are available, to the knowledge of the authors, in support of the predictions for materials having degenerate electron concentration. The lack of experimental results emanates from the difficulty of the measurement of the diffusion constant D for degenerate materials.

In this context, we wish to note that tetragonal materials are being increasing used in non-linear optics and light emitting devices [21]. Rowe and Shay [22] have demonstrated that the quasi-cubic model can be used to explain the observed splitting and symmetry properties of the conduction and valence bands at the zone centre in $\mathbf{k}$-space for such compounds. The s-like conduction band is singly degenerate and the p-like valence band is triply degenerate. Incorporating the anisotropic crystal potential into the Hamiltonian and the special features of the non-linear optical compounds, Kildal [23] proposed an energy spectrum for the conduction electrons under the assumptions of an isotropic momentum matrix element and isotropic spin–orbit splitting although the anisotropies in the aforementioned band parameters are significant physical features of the said materials [24]. In this paper, in section 2.1, we shall study the DMR in QWs and QWWs of tetragonal compounds, including the combined influence of the anisotropies of the said energy band constants and including the crystal field splitting.

It is worth remarking that III–V compounds are being increasingly used in integrated optoelectronics [25], photorefractive materials [26], distributed feedback lasers [27] and infrared photodetectors [28]. The three-band model of Kane [11] is valid for III–V, ternary and quaternary materials and must be used for studying the transport properties of n-InAs where the spin–orbit splitting constant is of the order of band gap. We shall study the DMR in QWs and QWWs of III–V semiconductors in section 2.2 of this paper. We shall show that the results for III–V quantum confined systems form special cases of our generalized analysis, as presented in section 2.1, under certain limiting conditions. In section 2.2, we shall also consider the simplified cases of the two-band model of Kane and that of wide gap semiconductors. It may be noted that the two-band model of Kane and parabolic energy bands can be derived from the three-band model of Kane under certain limiting conditions.

The II–VI compounds are suitable for use in optoelectronics [29], advanced microwave devices, light emitting diodes and infrared detectors [30]. The carriers of II–VI materials are defined by the Hopfield model [31] where the splitting of the two-spin states by the spin–orbit coupling and the crystalline field has been taken into account to describe the carrier energy spectra of these materials. In section 2.3, we shall study the DMR in QWs and QWWs of II–VI compounds on the basis of the Hopfield model by formulating the appropriate carrier statistics.

The IV–VI compounds find extensive applications in infrared detectors, thermoelectric devices, superlattices and quantum confined materials [32]. The dispersion relation of the carriers of IV–VI materials has been formulated by Cohen [33] by including band non-parabolicity and the anisotropies of the effective masses of the carriers. In section 2.4, we shall study the DMR in QWs and QWWs in IV–VI materials on the basis of the Cohen model. We shall show that, under certain limiting conditions, all the results for all the models will be reduced to the QWs and QWWs of relatively wide gap materials, which are well known in the literature [15]. The above statement highlights the compatibility of our mathematical formulation. In section 2.5, we shall suggest an experimental method for determining the DMR in materials having arbitrary dispersion laws. The effects of carrier degeneracy and the nanothickness on the DMR in QWs and QWWs of tetragonal III–V, II–VI and IV–VI compounds have been studied by taking n-CdGeAs$_2$, InAs, CdS and PbSe as examples for numerical computations.

2. Theoretical background

2.1. The formulations of the DMRs in QWs and QWWs of tetragonal materials on the basis of a newly formulated electron dispersion law

The form of the $\mathbf{k}\cdot\mathbf{p}$ matrix for the tetragonal compounds can be written as

$$H = \begin{bmatrix} H_1 & H_2 \\ H_2^+ & H_1 \end{bmatrix} \tag{1}$$

where

$$H_1 = \begin{bmatrix} E_g & P_\parallel k_z & 0 & 0 \\ P_\parallel k_z & -(\delta + (1/3)\Delta_\parallel) & (2\Delta_\perp/3) & 0 \\ 0 & (2\Delta_\perp/3) & -(2\Delta_\parallel/3) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

and

$$H_2 = \begin{bmatrix} 0 & 0 & f_{,-} & f_{,+} \\ 0 & 0 & 0 & 0 \\ -f_{,-} & 0 & 0 & 0 \\ f_{,+} & 0 & 0 & 0 \end{bmatrix}$$

in which E_g is the band gap, $P_\parallel$ and $P_\perp$ are the momentum matrix elements parallel and perpendicular to the direction of the **c** axis, respectively, δ is the crystal field splitting constant, $\Delta_\parallel$ and $\Delta_\perp$ are the spin–orbit splitting parameters parallel and perpendicular to the direction of the **c** axis, respectively,

$$f_\pm \equiv (P_\perp/\sqrt{2})(k_x \pm \mathrm{i}k_y) \qquad \text{and} \qquad \mathrm{i} = \sqrt{-1}.$$

Diagonalizing the above matrix, the generalized electron energy spectrum in the bulk specimens of the tetragonal materials can be expressed as

$$\gamma(E) = f_1(E)k_s^2 + f_2(E)k_z^2 \tag{2}$$

where

$$\begin{aligned}
\gamma(E) &\equiv \{E(E+E_g)[(E+E_g)(E+E_g+\Delta_\parallel) \\
&\quad + \delta(E+E_g+(1/3)\Delta_\parallel)] \\
&\quad + (2/9)E(E+E_g)(\Delta_\parallel^2-\Delta_\perp^2)\}, \qquad k_s^2 \equiv k_x^2 + k_y^2, \\
f_1(E) &\equiv \{\hbar^2 E_g(E_g+\Delta_\perp)[2m_\perp^*(E_g+(2/3)\Delta_\perp)]^{-1}\} \\
&\quad \times [\delta(E+E_g+(1/3)\Delta_\parallel) + (E+E_g)(E+E_g+(2/3)\Delta_\parallel) \\
&\quad + (2/9)(\Delta_\parallel^2-\Delta_\perp^2)], \\
f_2(E) &= \{\hbar^2 E_g(E_g+\Delta_\parallel)[2m_\parallel^*(E_g+(2/3)\Delta_\parallel)]^{-1}\} \\
&\quad \times [(E+E_g)(E+E_g+(2/3)\Delta_\parallel)]
\end{aligned}$$

in which E is the electron energy as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization, $\hbar = h/2\pi$, h is the Planck constant and $m_\parallel^*$ and $m_\perp^*$ are the effective masses of the electron at the edge of the conduction band parallel and perpendicular to the direction of the **c** axis, respectively.

The dispersion relations of the conduction electrons in QWs and QWWs of tetragonal materials can, respectively, be written as

$$\gamma(E) = f_1(E)k_s^2 + f_2(E)(\pi n_z/d_z)^2 \tag{3}$$

and

$$\gamma(E) = f_1(E)k_x^2 + f_1(E)(\pi n_y/d_y)^2 + f_2(E)(\pi n_z/d_z)^2 \tag{4}$$

where n_y $(=1, 2, 3, \ldots)$ and n_z $(=1, 2, 3, \ldots)$ are the size quantum numbers along the y and z directions respectively and d_y and d_z are the corresponding nanothicknesses along the y and z directions respectively. The carrier statistics in QWs and QWWs can, respectively, be expressed as

$$n_0 = (2\pi)^{-1}C_1[L_1(E_F) + L_2(E_F)] \tag{5}$$

and

$$n_0 = (2/\pi)C_2[L_3(E_F) + L_4(E_F)] \tag{6}$$

where

$$C_1 \equiv \sum_{n_z=1}^{n_{z\,\max}},$$

$$L_1(E_F) \equiv [[\gamma(E_F) - f_2(E_F)(\pi n_z/d_z)^2]/f_1(E_F)],$$

$$L_2(E_F) \equiv C_3k_1, \qquad C_3 \equiv \sum_{r=1}^{s},$$

$$k_i \equiv (k_BT)^{2r}(1-2^{1-2r})\zeta(2r)\frac{\partial^{2r}}{\partial E_F^{2r}}[L_i(E_F)],$$

$\zeta(2r)$ is the zeta function of order $2r$,

$$\begin{aligned}
L_3(E_F) &\equiv [[\gamma(E_F) - f_1(E_F)(\pi n_y/d_y)^2 \\
&\quad - f_2(E_F)(\pi n_z/d_z)^2]\{f_1(E_F)\}^{-1}]^{1/2},
\end{aligned}$$

$$L_4(E_F) \equiv C_3k_3, \qquad C_2 \equiv \sum_{n_y=1}^{n_{y\,\max}}\sum_{n_z=1}^{n_{z\,\max}}$$

and E_F is the corresponding Fermi energy.

Following Bouchaud and Georges [20], the DMR can be expressed as

$$\frac{D}{\mu} = \frac{n_0}{e}\left[\sum_i n_i\mu_i\theta_i^{-1}\right]\left[\sum_i n_i\mu_i\right]^{-1} \tag{7a}$$

where $\theta_i = \sum_j(\partial n_i(E_{Fj})/\partial E_{Fj})(\partial E_{Fj}/\partial E_{Fi})$, n_i and μ_i are the carrier concentration and the electron mobility for the ith band, respectively, $E_{Fi} = E_F - E_i$ and E_i is the energy of the subband. For the present case, $i = j = 0$ and E_i is independent of z. Thus (7a) gets simplified to

$$D/\mu = (n_0/e)\Big/\left(\frac{\partial n_0}{\partial E_F}\right). \tag{7b}$$

Therefore, we can combine (5), (6) and (7b) to get the respective expressions for the DMR in QWs and QWWs of tetragonal compounds as

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_1[L_1(E_F) + L_2(E_F)]}{C_1[L_1'(E_F) + L_2'(E_F)]}\right] \tag{8}$$

and

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_2[L_3(E_F) + L_4(E_F)]}{C_2[L'_3(E_F) + L'_4(E_F)]}\right] \tag{9}$$

respectively where the primes denote the differentiation of the respective differentiable functions with respect to the Fermi energy.

2.2. The formulations of the DMRs in QWs and QWWs of III–V materials as special cases of section 2.1

(i) Under the conditions $\Delta_\parallel = \Delta_\perp = \Delta$ (the isotropic spin–orbit splitting constant), $\delta = 0$ and $m^*_\parallel = m^*_\perp = m^*$ (the isotropic effective electron mass at the edge of the conduction band), (2) assumes the form

$$\frac{\hbar^2 k^2}{2m^*} = \frac{E(E+E_g)(E+E_g+\Delta)(E_g+(2/3)\Delta)}{E_g(E_g+\Delta)(E+E_g+(2/3)\Delta)}. \tag{10}$$

The above equation is the well-known three-band model of Kane [11], which is a valid model for studying the electronic properties of III–V, ternary and quaternary materials. Thus the expressions for n_0 and the DMR for QWs and QWWs of III–V materials can, respectively, be written, from (5), (8) and (6), (9) with the aforementioned substitutions, as

$$n_0 = (m^*/\pi\hbar^2)C_1[L_5(E_F) + L_6(E_F)], \tag{11}$$

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_1[L_5(E_F) + L_6(E_F)]}{C_1[L'_5(E_F) + L'_6(E_F)]}\right], \tag{12}$$

$$n_0 = (4\sqrt{2m^*}/h)C_2[L_7(E_F) + L_8(E_F)] \tag{13}$$

and

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_2[L_7(E_F) + L_8(E_F)]}{C_2[L'_7(E_F) + L'_8(E_F)]}\right] \tag{14}$$

where

$$L_5(E_F) \equiv \left[\frac{E_F(E_F+E_g)(E_F+E_g+\Delta)(E_g+(2/3)\Delta)}{E_g(E_g+\Delta)(E_F+E_g+(2/3)\Delta)} - \left(\frac{\hbar^2\pi^2}{2m^*}\right)\left(\frac{n_z}{d_z}\right)^2\right],$$

$$L_6(E_F) \equiv C_3 k_5,$$

$$L_7(E_F) \equiv \left[L_5(E_F) - \left(\frac{\hbar^2\pi^2}{2m^*}\right)\left(\frac{n_y}{d_y}\right)^2\right]^{1/2}$$

and

$$L_8(E_F) \equiv C_3 k_7.$$

(ii) Under the conditions $\Delta \gg E_g$ or $\Delta \ll E_g$, (10) assumes the form

$$E(1+\alpha E) = \hbar^2 k^2/2m^*, \qquad \alpha \equiv 1/E_g, \tag{15}$$

which is known as the simplified two-band model of Kane and is often used to study the transport properties of III–V materials excluding n-InAs [11]. Thus with these inequalities, (11)–(14) get simplified to

$$n_0 = (m^*/\pi\hbar^2)C_1[L_9(E_F) + L_{10}(E_F)], \tag{16}$$

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_1[L_9(E_F) + L_{10}(E_F)]}{C_1[L'_9(E_F) + L'_{10}(E_F)]}\right], \tag{17}$$

$$n_0 = (4\sqrt{2m^*}/h)C_2[L_{11}(E_F) + L_{12}(E_F)] \tag{18}$$

and

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_2[L_{11}(E_F) + L_{12}(E_F)]}{C_2[L'_{11}(E_F) + L'_{12}(E_F)]}\right] \tag{19}$$

where

$$L_9(E_F) \equiv \left[E_F(1+\alpha E_F) - (\hbar^2\pi^2/2m^*)\left(\frac{n_z}{d_z}\right)^2\right],$$

$$L_{10}(E_F) \equiv C_3 k_9,$$

$$L_{11}(E_F) \equiv \left[L_9(E_F) - (\hbar^2\pi^2/2m^*)\left(\frac{n_y}{d_y}\right)^2\right]^{1/2}$$

and

$$L_{12}(E_F) \equiv C_3 k_{11}.$$

(iii) For wide gap materials, $E_g \to \propto$ and the expressions for n_0 and the DMR for QWs and QWWs of relatively wide gap materials having parabolic energy bands assume the forms [15]

$$n_0 = \left(\frac{m^* k_B T}{\pi\hbar^2}\right)C_1[F_0(\eta_1)], \tag{20}$$

$$\frac{D}{\mu} = (k_B T/e)C_1[F_0(\eta_1)]/C_1[F_{-1}(\eta_1)], \tag{21}$$

$$n_0 = \frac{2}{h}\sqrt{2\pi m^* k_B T}\,C_2[F_{-1/2}(\eta_2)] \tag{22}$$

and

$$\frac{D}{\mu} = (k_B T/e)C_2[F_{-1/2}(\eta_2)]/C_2[F_{-3/2}(\eta_2)] \tag{23}$$

where

$$\eta_1 \equiv \left[E_F - \left(\frac{\hbar^2}{2m^*}\right)(\pi n_z/d_z)^2\right]\Big/ k_B T,$$

$$\eta_2 \equiv \left[\eta_1 - \left(\frac{\hbar^2\pi^2}{2m^* k_B T}\right)(n_y/d_y)^2\right]$$

and $F_t(\eta)$ is the Fermi–Dirac integral parameter of order t [34, 35] which can be defined as

$$F_t(\eta) = (\Gamma(t+1))^{-1}\int_0^\infty x^t[1+\exp(x-\eta)]^{-1}\,\mathrm{d}x \quad \text{for } t > -1 \tag{24}$$

or, for all t, analytically continued as a complex contour integral around the negative x axis as

$$F_1(\eta) = (\Gamma(-t)/2\pi\sqrt{-1})\int_{-\infty}^{0} x^t[1+\exp(-x-\eta)]^{-1}\,\mathrm{d}x. \tag{25}$$

Under the condition of non-degenerate carrier concentration, (21) and (23) lead to the well-known result giving the DMR as $(D/\mu) = k_B T/e$ [6] which shows that the result is independent of the quantum confinement.

2.3. The formulations of the DMRs in QWs and QWWs of II–VI materials

The energy spectra of both the carriers of II–VI compounds can be expressed as [31]

$$E = Ak_s^2 + Bk_z^2 + Ck_s \tag{26}$$

where $A \equiv \hbar^2/2m_\perp^*$, $B \equiv \hbar^2/2m_\parallel^*$ and C represents the splitting of the two spin states by the spin–orbit coupling and the crystalline field. The carrier statistics in QWs and QWWs of II–VI compounds can, respectively, be written as

$$n_0 = (16\pi A^2)^{-1}[C_1[L_{13}(E_{\mathrm{F}}) + L_{14}(E_{\mathrm{F}})]] \tag{27}$$

and

$$n_0 = (\pi)^{-1}[C_2[L_{15}(E_{\mathrm{F}}) + L_{16}(E_{\mathrm{F}})]] \tag{28}$$

where

$$L_{13}(E_{\mathrm{F}}) \equiv [2C^2 - 4AB(\pi n_z/d_z)^2 + 4AE_{\mathrm{F}} \pm 2C\{C^2 - 4AB(\pi n_z/d_z)^2 + 4AE_{\mathrm{F}}\}^{1/2}],$$

$$L_{14}(E_{\mathrm{F}}) \equiv C_3 k_{13},$$

$$L_{15}(E_{\mathrm{F}}) \equiv [(4A^2)^{-1}L_{13}(E_{\mathrm{F}}) - (\pi n_y/d_y)^2]^{1/2}$$

and

$$L_{16}(E_{\mathrm{F}}) \equiv C_3 k_{15}.$$

Thus combining (7*b*), (27) and (28), we get that the DMRs in QWs and QWWs of II–VI compounds can, respectively, be expressed as

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_1[L_{13}(E_{\mathrm{F}}) + L_{14}(E_{\mathrm{F}})]}{C_1[L'_{13}(E_{\mathrm{F}}) + L'_{14}(E_{\mathrm{F}})]}\right] \tag{29}$$

and

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_2[L_{15}(E_{\mathrm{F}}) + L_{16}(E_{\mathrm{F}})]}{C_2[L'_{15}(E_{\mathrm{F}}) + L'_{16}(E_{\mathrm{F}})]}\right]. \tag{30}$$

Under the conditions $A = B = \hbar^2/2m^*$ and $C \to 0$, (29) and (30) get simplified to (21) and (23) respectively.

2.4. The formulations of the DMRs in QWs and QWWs of IV–VI materials

The electron dispersion law in IV–VI compounds can be expressed in accordance with Cohen [33] as

$$E(1 + \alpha E) = p_x^2/2m_1 + p_y^2/2m_2 + p_z^2/2m_3 + \frac{\alpha E p_y^2}{2}\left(\frac{1}{m_2} - \frac{1}{m'_2}\right) - \frac{\alpha p_y^4}{4m_2 m'_2} \tag{31}$$

where m_1 and m_3 are the band-edge effective electron masses in the transverse directions, m_2 is the band-edge effective electron mass in the longitudinal direction and m'_2 is the longitudinal band-edge effective mass of the holes. The carrier statistics in QWs and QWWs of IV–VI materials can, respectively, be expressed as

$$n_0 = (g_v\sqrt{m_1 m_3}/\pi\hbar^2)\sum_{n_y=1}^{n_{y\max}}[L_{17}(E_{\mathrm{F}}) + L_{18}(E_{\mathrm{F}})] \tag{32}$$

and

$$n_0 = (2g_v\sqrt{2m_1}/\pi\hbar)C_2[L_{19}(E_{\mathrm{F}}) + L_{20}(E_{\mathrm{F}})] \tag{33}$$

where g_v stands for valley degeneracy

$$L_{17}(E_{\mathrm{F}}) \equiv [E_{\mathrm{F}}(1 + \alpha E_{\mathrm{F}}) - (\hbar^2/2m_2)(\pi n_y/d_y)^2 - (\alpha E_{\mathrm{F}}\hbar^2\pi^2/2)(n_y/d_y)^2[(m_2)^{-1} - (m'_2)^{-1}] - (\alpha\hbar^4\pi^4/4m_2m'_2)(n_y/d_y)^4],$$

$$L_{18}(E_{\mathrm{F}}) \equiv C_3 k_{17},$$

$$L_{19}(E_{\mathrm{F}}) \equiv [L_{17}(E_{\mathrm{F}}) - (\hbar^2\pi^2/2m_3)(n_z/d_z)^2]^{1/2}$$

and

$$L_{20}(E_{\mathrm{F}}) \equiv C_3 k_{19}.$$

Using (7*b*), (32) and (33), the DMRs in QWs and QWWs of IV–VI compounds can, respectively, be expressed as

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{\sum_{n_y=1}^{n_{y\max}}[L_{17}(E_{\mathrm{F}}) + L_{18}(E_{\mathrm{F}})]}{\sum_{n_y=1}^{n_{y\max}}[L'_{17}(E_{\mathrm{F}}) + L'_{18}(E_{\mathrm{F}})]}\right] \tag{34}$$

and

$$\frac{D}{\mu} = (e)^{-1}\left[\frac{C_2[L_{19}(E_{\mathrm{F}}) + L_{20}(E_{\mathrm{F}})]}{C_2[L'_{19}(E_{\mathrm{F}}) + L'_{20}(E_{\mathrm{F}})]}\right]. \tag{35}$$

Under the conditions $\alpha \to 0$ and $m_1 = m_2 = m_3 = m^*$, (34) and (35) get simplified to (21) and (23) respectively.

2.5. An experimental suggestion for the determination of the DMR in degenerate materials having arbitrary dispersion laws

It is well known that in the presence of a large magnetic field, the thermoelectric power is determined only by the dispersion laws [36]. The magnitude of the thermoelectric power for the present system can be written as [36]

$$L_0 = \left(\frac{1}{eTn_0}\right)\int_{-\infty}^{\infty}(E - E_{\mathrm{F}})R(E)\left[-\frac{\partial f_0}{\partial E}\right]\mathrm{d}E \tag{36}$$

where $R(E)$ is the total number of states and f_0 is the Fermi–Dirac distribution function. Following Tsidilkovski [37], (36) can be expressed as

$$L_0 = (\pi^2 k_{\mathrm{B}}T/3en_0)\left(\frac{\partial n_0}{\partial E_{\mathrm{F}}}\right). \tag{37}$$

Using (7*b*) and (37), we get

$$\frac{D}{\mu} = \pi^2 k_{\mathrm{B}}T/3L_0 e^2. \tag{38}$$

Therefore, we can, experimentally, determine the DMR for any degenerate material having an arbitrary dispersion law by knowing L_0, which is an easily measurable experimentally quantity.

Thus we can summarize the whole theoretical background in the following way.

In this paper we have formulated the expressions for the carrier statistics in QWs and QWWs of tetragonal (on the basis of a new dispersion law), III–V (a special case of the above), II–VI and IV–VI compounds without any approximations regarding the respective energy band constants, from which we have obtained the corresponding DMRs. The results of the three-band and the two-band models of Kane have formed special cases of our generalized analysis. Also, under certain limiting conditions, all the models reduce to the

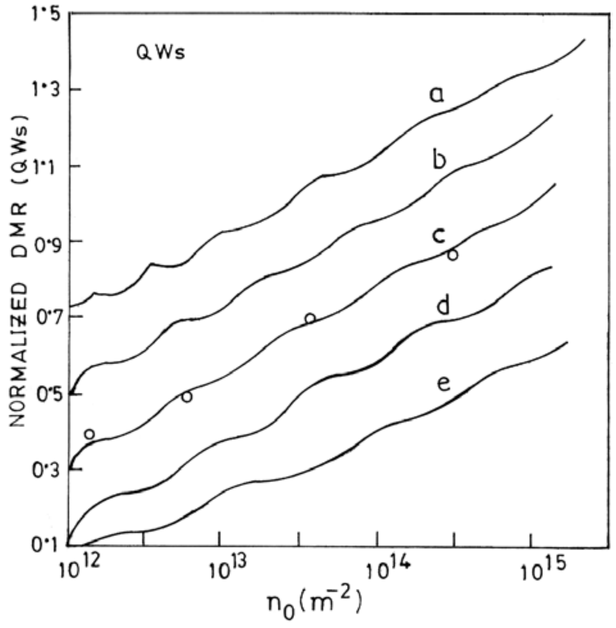

Figure 1. A plot of the normalized DMR at 4.2 K as a function of surface electron concentration per unit area in QWs: (a) $CdGeAs_2$; (b) $\delta = 0$; (c) InAs; (d) CdS; (e) PbSe ($d_z = 40$ nm). The circular plot was obtained using (38) together with the experimental results on L_0 versus n_0 as given in [38].

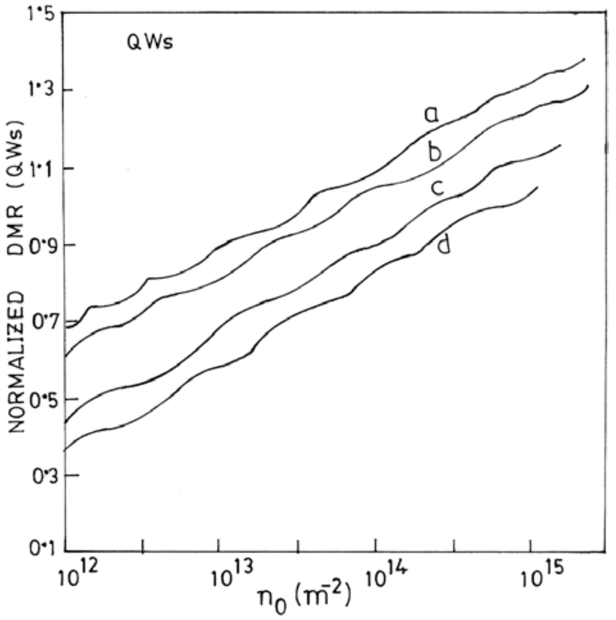

Figure 2. A plot of the normalized DMR at 4.2 K as a function of the surface electron concentration per unit area in QWs of $CdGeAs_2$ for: (a) $m^*_\parallel = m^*_\perp$ and $\delta \neq 0$; (b) $m^*_\parallel = m^*_\perp$ and $\delta = 0$; (c) $\Delta_\parallel = \Delta_\perp$ and $\delta \neq 0$; (d) $\Delta_\parallel = \Delta_\perp$ and $\delta = 0$.

well-known results of the DMRs for QWs and QWWs for relatively wide gap materials having parabolic energy bands. The above statement provides an indirect theoretical test of our mathematical analysis. In addition, we have suggested a dimension independent experimental method for determining the DMR in degenerate materials having arbitrary dispersion laws.

3. Results and discussion

Using (5) and (8) together with the parameters [21] $\Delta_{11} = 0.30$ eV, $\Delta_\perp = 0.36$ eV, $m^*_{11} = 0.035\, m_0$, $m^*_\perp = 0.039\, m_0$, $\delta = -0.21$ eV, $E_g = 0.57$ eV, $d_z = 20$ nm and $T = 4.2$ K, we have plotted in figure 1 the normalized DMR in QWs of $CdGeAs_2$ versus surface electron concentration as shown by curve (a); curve (b) shows the same dependence for $\delta = 0$ so that we can assess the influence of crystal field splitting on the DMR for the present case. Taking the parameters $\Delta = 0.43$ eV, $m^* = 0.026\, m_0$ and $E_g = 0.36$ eV at 4.2 K [11] and using (11) and (12) we have plotted the normalized DMR in QWs of n-InAs as a function of n_0 as shown by curve (c) of figure 1, where the circular plot has been obtained by using (38) and the experimental results of $\mathbf{L}_0$ versus $\mathbf{n}_0$ for QWs of n-InAs as given in [38]. Plot (d) of figure 1 is for QWs of CdS and has been obtained by using (27) and (29) together with the parameters [39] $m^*_{11} = 0.7\, m_0$, $m^*_\perp = 1.5\, m_0$, $T = 4.2$ K and $C = 1.47 \times 10^{-10}$ eV m. Plot (e) of figure 1 has been drawn for QWs of n-PbSe; it was obtained by using (32) and (34) with $m_1 = m_3 = 0.04\, m_0$, $T = 4.2$ K, $m_2 = 0.07\, m_0$, $m'_2 = 0.068\, m_0$, $E_g = 0.15$ eV at 4.2 K taken as the band parameters of n-PbSe [10].

In figure 2 we have plotted as graph (a) the normalized DMR at 4.2 K as a function of the surface electron concentration per unit area in QWs of $CdGeAs_2$, taking $m^*_\parallel = m^*_\perp$ and $\delta \neq 0$; plot (b) represents the same case but for $m^*_\parallel = m^*_\perp$ and $\delta = 0$. Curve (c) has been drawn for $\Delta_\parallel = \Delta_\perp$ but $\delta \neq 0$ whereas curve (d) is for $\Delta_\parallel = \Delta_\perp$ but $\delta = 0$. Thus by comparing figures 1 and 2 we can easily assess the influence of the anisotropies of the individual band parameters on the DMR for QWs of $CdGeAs_2$.

In figure 3 all the cases of figure 1 have been plotted for QWWs as functions of the electron concentration per unit length by using the appropriate equations. In figure 4 we have plotted as curve (a) the normalized DMR at 4.2 K as a function of the surface electron concentration per unit length in QWWs of $CdGeAs_2$, taking $m^*_\parallel = m^*_\perp$ and $\delta \neq 0$; curve (b) of figure 4 represents the same case but for $m^*_\parallel = m^*_\perp$ and $\delta = 0$. Curve (c) has been drawn for $\Delta_\parallel = \Delta_\perp$ but $\delta \neq 0$ whereas curve (d) is for $\Delta_\parallel = \Delta_\perp$ but $\delta = 0$. Thus by comparing figures 3 and 4 we can easily assess the influence of the anisotropies of the individual band parameters on the DMR for QWWs of $CdGeAs_2$.

From figures 1 and 3 we observe that the DMR oscillates with n_0 in different manners which are characteristic features of the dimension reduction. The oscillatory dependence is influenced by the crossing of the Fermi level by size-quantized levels in steps. Since the Fermi energy in quantum confined materials is an oscillatory function of n_0 and film thickness and also since the DMR is a function of E_F, the DMR oscillates with n_0 and the film thickness. From curves (a) and (b) of figure 1 it appears that the presence of a crystal field splitting constant enhances the numerical value of the DMR in QWs of $CdGeAs_2$. From figures 1 and 3 it appears that the numerical values of the DMRs are greatest for $CdGeAs_2$ and least for PbSe for all types of quantum confined material as considered here, taking into account the fact that the values of the DMRs in the QWWs are larger than those for the QWs. This fact is a consequence of the dispersion relations of the materials and the appropriate dimension reduction.

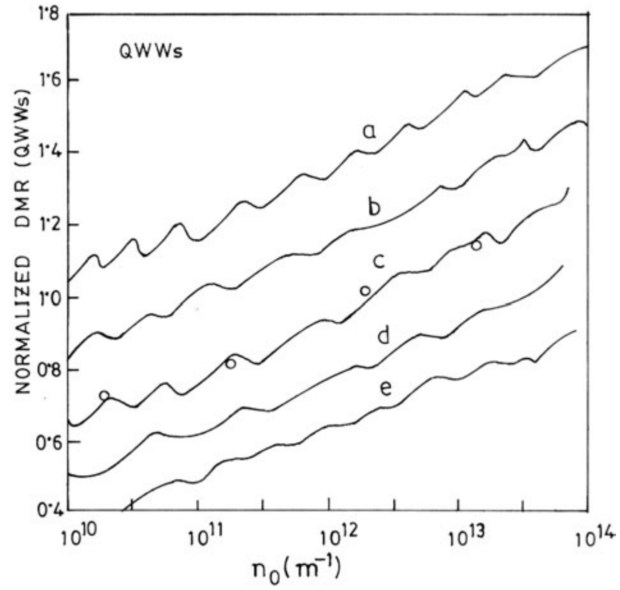

Figure 3. A plot of the normalized DMR at 4.2 K as a function of the electron concentration per unit length in QWs: (a) $CdGeAs_2$; (b) $\delta = 0$; (c) InAs; (d) CdS; (e) PbSe ($d_z = 40$ nm). The circular plot was obtained using (38) together with the experimental results on L_0 versus n_0 as given in [38].

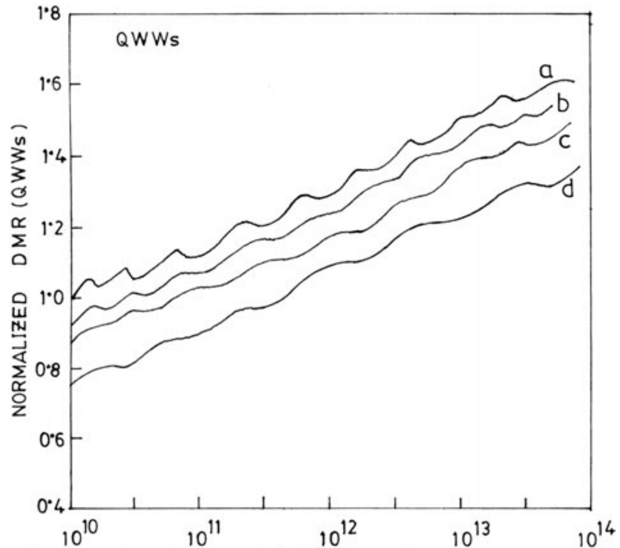

Figure 4. A plot of the normalized DMR at 4.2 K as a function of the surface electron concentration per unit length in QWWs of $CdGeAs_2$ for: (a) $m^*_\parallel = m^*_\perp$ and $\delta \neq 0$; (b) $m^*_\parallel = m^*_\perp$ and $\delta = 0$; (c) $\Delta_\parallel = \Delta_\perp$ and $\delta \neq 0$; (d) $\Delta_\parallel = \Delta_\perp$ and $\delta = 0$.

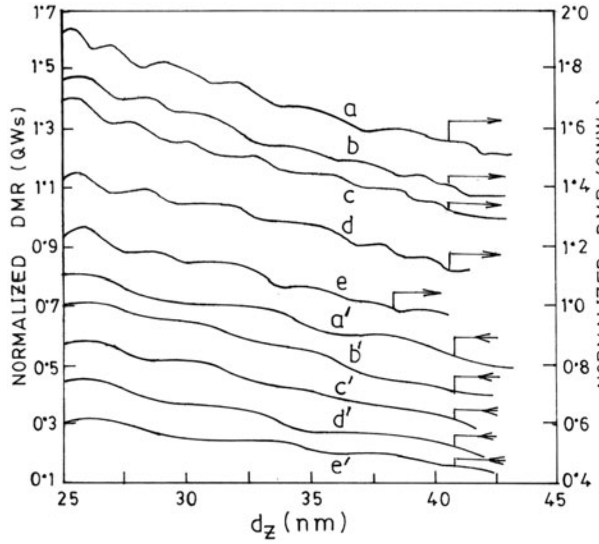

Figure 5. A plot of the normalized DMRs for cases (a)–(e) of figure 1 for both QWs and QWWs ($d_y = 30$ nm) as a function of d_z ($n_0 = 10^{17}$ m^{-2} for QWs and $n_0 = 10^{15}$ m^{-1} for QWWs).

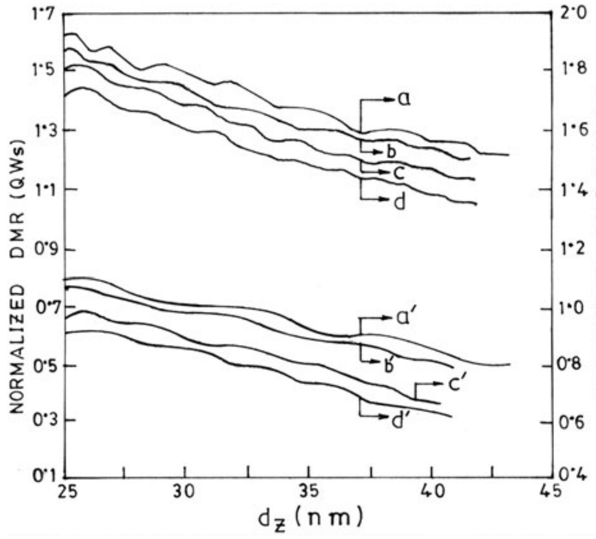

Figure 6. A plot of the normalized DMR at 4.2 K as a function of d_z in QWs of $CdGeAs_2$ for: (a) $m^*_\parallel = m^*_\perp$ and $\delta \neq 0$; (b) $m^*_\parallel = m^*_\perp$ and $\delta = 0$; (c) $\Delta_\parallel = \Delta_\perp$ and $\delta \neq 0$; (d) $\Delta_\parallel = \Delta_\perp$ and $\delta = 0$. The plots (a′)–(d′) show the same dependences for the QWWs of $CdGeAs_2$.

The influence of quantum confinement is immediately apparent from figure 5 since the DMR depends strongly on the thickness of the quantum confined systems in direct contrast with the case for the bulk specimens of the said compounds. The DMR exhibits a strong oscillatory dependence on the thickness. The appearance of the humps in figure 5 is due to the redistribution of the electrons amongst the quantized energy levels when the size quantum number corresponding to the highest occupied level changes from one fixed value to another. The DMR in quantum confined materials can become several orders of magnitude larger than that in the bulk specimens of the same materials, which is also a direct consequence of system asymmetry arising through dimensional reduction. By comparing figures 5 and 6 we can easily assess the influence of anisotropic band constants on the DMR for QWs and QWWs of $CdGeAs_2$ with respect to the film thickness.

It may be noted that the DMR is connected to $\partial n_0/\partial E_F$ as given by (7*b*). Our experimental suggestion for the determination of the DMR for materials having arbitrary dispersion laws does not contain any band parameter. For constant temperature, the DMR (D/μ) varies inversely with L_0. Only the experimental values of L_0 for any material as a function of electron concentration will give the experimental values of the DMR for that range of n_0. Since the experimental values L_0 in the present case are not available in the literature to the best of our knowledge (except for n-InAs), our theoretical formulation cannot be compared with the proposed experiment for the other types of quantum confined system considered here. Since L_0 decreases with doping in an oscillatory way, from (38) we can conclude that the DMR will increase with increasing n_0 in an oscillatory manner, as is also evident from figures 1 and 3. This statement provides a compatibility test of our theoretical analysis.

Equation (38) provides an experimental check of the DMR and also a technique for probing the band structures of quantum confined materials. We wish to note that we have not considered the hot electron and many-body effects in this simplified theoretical formalism due to the lack of availability in the literature of the proper analytical techniques for including them for the generalized systems considered in this paper. Our simplified approach will be useful for the purpose of comparison when methods for tackling the formidable problem of inclusion of the many-body and hot electron effects for the present generalized systems appear. It is worth remarking in this context that our simplified theoretical results for the DMRs in QWs and QWWs of n-InAs are in quantitative agreement with the suggested experimental method of determining the DMR for materials having arbitrary band structures, even in the absence of consideration of the many-body and hot electron effects. The inclusion of these effects would certainly increase the accuracy of the results, although our suggestion for the experimental determination of the DMR is independent of the inclusion of the said effects and the qualitative features of the DMR discussed in this paper would not change in the presence of the aforementioned effects.

In this paper, we studied, in section 2.1, the DMR in QWs and QWWs of tetragonal materials using n-CdGeAs$_2$ as an example. In formulating the expressions for the DMRs in such quantum confined materials, we have considered the crystal field splitting, the anisotropies of the effective electron masses and spin–orbit splitting parameters, since these are the significant physical features of such non-linear optical compounds [24]. In the absence of crystal field splitting, and with the assumptions of isotropic effective electron mass and spin–orbit splitting, the expressions for the quantum confined DMRs as given by (8) and (9) convert into the corresponding equations (12) and (14) as given in section 2.2. Equations (12) and (14) are valid for QWs and QWWs of III–V, ternary and quaternary compounds whose energy band structures are defined by the three-band model of Kane. For many important aforementioned materials, $\Delta \gg E_{\mathrm{g}}$ or $\Delta \ll E_{\mathrm{g}}$. With these inequalities, (12) and (14) should, respectively, be replaced by (17) and (19). For semiconductors having parabolic energy bands, (17) and (19) get transformed into (21) and (23) respectively. In addition, for non-degenerate electron concentration, (21) and (23) reduce to the well-known result $(D/\mu) = k_{\mathrm{B}}T/e$ as noted already and derived for the first time by Einstein. Thus our generalized formulation covers various materials under different conditions of quantum confinement.

In section 2.3 we studied the DMRs in QWs and QWWs of II–VI materials in accordance with the Hopfield model, where the splitting of the two spin states by the spin–orbit coupling and crystalline field has been taken into account in describing the carrier energy spectrum in II–VI compounds. In section 2.4 we studied the corresponding DMRs for IV–VI quantum confined compounds on the basis of the Cohen model. It may be noted that the Cohen model is also used to study the transport properties of bismuth. The importance of bismuth with respect to the experimental and theoretical realization of quantum confinement is already well known in the literature [40]. Our study is also valid for QWs and QWWs of bismuth with the proper changes in the energy band constants. In section 2.5 we suggested that the DMR varies inversely with the thermoelectric power for the present system when temperature is kept constant. This suggestion is again dimension independent.

It is worth remarking that the influence of energy band models on the DMR in quantum confined materials can be assessed from this work and this simplified analysis also covers various dimensionally reduced compounds in the quantum regime having different dispersion relations. We have not considered other types of quantum confined materials or other physical variables for plotting the DMR for the purpose of maintaining a condensed presentation. The variations of the DMRs are totally band structure dependent. It may be remarked that in recent years, the mobilities of the quantum confined compounds have been extensively studied, but the diffusion constants in such materials have been less fully investigated. Thus the result of our paper can be used for the determination of the diffusion constants in QWs and QWWs of tetragonal, III–V, II–VI and IV–VI materials by using the experimental values of the corresponding mobilities. Finally, it may be noted that the basic aim of this paper is not solely to study the DMR but also to formulate the electron concentration, since investigations of the different transport properties in QWs and QWWs are based on the temperature dependent carrier statistics in such materials having various dispersion relations.

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