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THE EINSTEIN RELATION IN SUPERLATTICES OF NON-PARABOLIC SEMICONDUCTORS WITH GRADED INTERFACES UNDER MAGNETIC QUANTIZATION

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We study the Einstein relation under magnetic quantization in III-V, II-VI, Pb-SnTe/PbTe, strained layer and HgTe/CdTe superlattices with graded interfaces and compare the same with that of the corresponding bulk specimens of the constituent materials. It is found, taking GaAs/$Ga_{1-x}Al_xAs$, CdS/CdTe, PbTe/PbSnTe, InAs/GaSb and HgTe/CdTe superlattices with graded interfaces as examples, that the Einstein relation exhibits oscillatory dependence with the inverse quantizing magnetic field due to the Shubnikov-de Haas effect, and increases with increasing electron concentration in an oscillatory manner in all the cases. The ratio of diffusivity to mobility in graded superlattices is greater than that of constituent bulk materials. The oscillations in HgTe/CdTe superlattices show up much more significantly as compared to other systems. In addition, we have suggested an experimental method of determining the Einstein relation in degenerate materials having arbitrary dispersion laws.

1. Introduction

With the advent of molecular beam epitaxy, fine line lithography and other experimental techniques [1], it has become possible to fabricate superlattices of non-parabolic semiconductors (hereafter referred to as SL's) composed of alternate layers of two different degenerate materials with controlled thicknesses, many of which are currently under study due to their interesting physical properties. The SL's, as orginally proposed by Esaki and Tsu [2], have found wide applications in many device structures, such as photodetectors, avalanche photodiodes [3], transistors [4], tunneling devices, light emitters [5] etc. The most extensively studied III-V SL is the one consisting of alternate layers of GaAs and $Ga_{1-x}Al_xAs$ owing to the relative ease in its fabrication. The GaAs layers form quantum wells and the $Ga_{1-x}Al_xAs$ layers form potential barriers. The III-V SL's are attractive for the realization of high-speed electronic and optoelectronic devices [6]. In addition to the SL's with the usual structure, superlattices with more complex structures such as PbTe/PbSnTe [7], II-VI [8],strained layer [9] and HgTe/CdTe [10] SL's have also been proposed. PbTe/PbSnTe SL exhibits quite different properties as compared to the III-V SL due to the peculiar band structure of the constituent materials [11]. The epitaxial growth of II-VI SL is a relatively recent development and the primary motivation for studying the mentioned SL's made of materials with the large band gap is in their potential for optoelectronic operation in the blue [11]. The strained layer SL's are of current interest both for scientific and device purposes [9]. HgTe/CdTe SL's have raised a great deal of attention since 1979 when they were first suggested as a promising new materials for long wavelength infrared detectors and other electro-optical applications [12]. Interest in Hg-based SL's has been further increased as new properties with potential device applications were revealed [12,13]. These features arise from the unique zero band gap material HgTe [14] and the direct band gap semiconductor CdTe which can be described by the three-band model of Kane [15]. The combination of the aforementioned materials with specified dispersion relation makes HgTe/CdTe SL very attractive, especially because of the possibility to tailor the material properties for various applications by varying the energy band constants of the SL.

We note that all the aforementioned SL's have been proposed with the assumption that the interfaces between the layers are sharply defined, of zero thickness, i.e. devoid of any interface effects. The SL potential distribution may be then considered as a one-dimensional array of rectangular potential wells. The aforementioned advanced experimental techniques may produce SL's with physical interfaces between two materials crystallographically abrupt, adjoining their interface will change at least on an atomic scale. As the potential form changes from a well (barrier) to a barrier (well), an intermediate potential region exists for the electrons. The influence of finite thickness of the interfaces on the electron dispersion law is very important since the electron energy spectrum governs the electron transport in SL's. In the present paper we shall study the Einstein relation for the diffusivity to mobility ratio of the electrons (hereafter referred to as DMR) in the aforementioned SL's with graded interfaces for the more interesting case which occurs from the presence of a quantizing magnetic field, and compare the same in the bulk specimens of the constituting materials by formulating the respective magneto-dispersion laws.

It is well-known that the DMR in semiconductors is a very useful quantity since the diffusion constant (a very important device parameter that can not be easily experimentally determined) can be derived from this relation using the experimental values of the mobility. Furthermore, the relation of the DMR with the velocity auto-correlation function [16], its modification due to non-linear charge transport [17], its relation to the screening length [18] and the different formulations of the DMR under various physical conditions have extensively been investigated [19-24]. Nevertheless, the DMR in narrow-gap SL's under magnetic quantization has yet to be derived.

We focus in this paper on Einstein relation because of its importance in the field of semiconductor science and technology and also in analyzing various types of electron devices. The III-V compound semiconductors find extensive applications in Bragg reflectors, distributed feedback lasers and photorefractive materials. The II-VI materials are suitable for light emitting diodes, optical fiber communications and advanced microwave devices. PbTe type materials find application in infrared lasers, optoelectronic devices and detectors. HgTe type gapless materials receive considerable attention in optoelectronics and infrared detection. In Section 2.1 we shall formulate the magneto DMR for the aforementioned SL's with graded interfaces and for the constituting materials, by formulating the electron statistics. In Section 2.2 we shall propose an experimental method of determining the DMR in degenerate materials having arbitrary dispersion laws. We shall study the doping and the magnetic field dependences of the DMR's, taking GaAs/$Ga_{1-x}Al_xAs$, PbTe/PbSnTe, CdS/CdTe, InAs/GaSb and HgTe/CdTe SL's with graded interfaces as examples.

2. Theoretical background

2.1. Formulation of magneto DMR in III-V SL's of non-parabolic materials with graded interface and the constituting compounds

The energy spectrum of the conduction electrons in bulk specimens of the constituting materials of III-V SL, whose energy band structures are described by the three-band Kane model, can be written [25], following Kane [15], as

$$\frac{\hbar^2 k^2}{2m_i^*} = EG(E, E_{gi}, \Delta_i) \tag{1}$$

where $\hbar = h/2\pi$, h is the Planck's constant, $\vec{k}$ is electronic wave vector, $i = 1,\ 2$, m_i^* is the effective electron mass at the edge of the conduction band, E is the total electron energy as measured from the edge of the conduction band in the absence of any quantization,

$$G(E, E_{gi}, \Delta_i) = \frac{(E + E_{gi})(E + E_{gi} + \Delta_i)(E_{gi} + 2\Delta_i/3)}{E_{gi}(E_{gi} + \Delta_i)(E + E_{gi} + 2\Delta_i/3)}, \qquad (2a)$$

E_{gi} is the band gap and Δ_i is the spin-orbit splitting of the valence band. The electron dispersion law in III-V SL with graded interface can be expressed, extending the method as given elsewhere [26], as

$$\cos(kl_0) = \frac{\phi(E)}{2} \qquad (2b)$$

where $l_0(= a_0 + b_0)$ is the period length, a_0 and b_0 are the widths of the barrier and well, respectively,

$$\phi(E) = \{2\cosh(\beta(E))\cos(\gamma(E)) + \epsilon(E)\sinh(\beta(E))\sin(\gamma(E)) + \Delta_0$$

$$\cdot \left[\left(\frac{K_0^2(E)}{K'(E)} - 3K'(E) \right) \cosh(\beta(E))\sin(\gamma(E)) + \left(3K_0(E) - \frac{K'^2(E)}{K_0(E)} \right) \cdot \sinh(\beta(E)) \right.$$

$$\cdot \cos(\gamma(E)) + 2\left(K_0^2(E) - K'^2(E) \right) \cosh(\beta(E))\cos(\gamma(E))$$

$$\left. + \frac{1}{12} \left(\frac{5K_0^3(E)}{K'(E)} + \frac{5K'^3(E)}{K_0(E)} - 34K_0(E)K'(E) \right) \sinh(\beta(E))\sin(\gamma(E)) \right] \Bigg\},$$

$$\epsilon(E) = \left[\frac{K_0(E)}{K'(E)} - \frac{K'(E)}{K_0(E)} \right], \quad \beta(E) = K_0(E)(a_0 - \Delta_0),$$

Δ_0 is the interface width,

$$K_0(E) = \left[2m_2^* \hbar^{-2} E' G(E - V_0, \alpha_2, \Delta_2) + k_\perp^2 \right]^{1/2},$$

$E' = (V_0 - E)$, V_0 is the potential barrier encountered by the electron, $\alpha_i = 1/E_{gi}$, $k_\perp^2 = k_x^2 + k_y^2$, $\gamma(E) = K'(E)(b_0 - \Delta_0)$ and

$$K'(E) = \left[2m_1^* \hbar^{-2} E G(E, \alpha_1, \Delta_1) - k_\perp^2 \right]^{1/2}.$$

In the presence of a quantizing magnetic field B along z-direction, the magneto-dispersion relation assumes the form,

$$l_0 k_z = \left[\rho(E,n) - 2eB\hbar^{-1} l_0^2 (n + \frac{1}{2})\right]^{1/2} \tag{3}$$

where $n(= 0, 1, 2, ...)$ is the Landau quantum number and the function $\rho(E, n)$ is defined in the Appendix A1. Considering the lowest mini-band, since in an actual SL only the lowest mini-band is significantly populated at low temperatures where the quantum effects become prominent, the relation between the electron concentration and the Fermi energy, taking the influence of broadening, can be written as

$$n_0 = \frac{eBg_v}{\pi^2 \hbar l_0} \sum_{n=0}^{n_{max}} [Q_1(n, E_F) + Q_2(n, E_F)] \tag{4}$$

where g_v is the valley degeneracy, $Q_1(n, E_F)$ = Real part of $[\rho(E_0, n) - 2eB\hbar^{-1} l_0^2 (n + \frac{1}{2})]^{1/2}$, $E_0 = E_F + \mathrm{i}\Gamma$, $\mathrm{i} = \sqrt{-1}$, Γ is the broadening of the Landau level and is given by $\Gamma = \pi k_B T_D$ in which T_D is Dingle temperature, k_B is the Boltzmann constant,

$$Q_2(n, E_F) = \sum_{r=1}^{S} Z_r(Q_1(n, E_F)),$$

r is the set of real positive integers, $Z_r = 2(k_B T)^{2r} \cdot (1 - 2^{1-2r})\zeta(2r) \mathrm{d}^{2r}/\mathrm{d}E_F^{2r}$, T is the temperature, $\zeta(2r)$ is the zeta function of order $2r$ and E_F is the Fermi energy.

The DMR of the electron can, in general, be written as [19]

$$\frac{D}{\mu} = \left(\frac{n_0}{e}\right) \Big/ \left(\frac{\partial n_0}{\partial E_F}\right). \tag{5}$$

Using Eqs. (4) and (5) we get

$$\frac{D}{\mu} = \frac{1}{e} \frac{\sum_{n=0}^{n_{max}} [Q_1(n, E_F) + Q_2(n, E_F)]}{\sum_{n=0}^{n_{max}} [Q_1'(n, E_F) + Q_2'(n, E_F)]} \tag{6}$$

where the primes denote the differentiation with respect to E_F.

We shall now derive an expression of the magneto DMR for bulk specimens of III-V materials by using Eq. (1). Under magnetic quantization, the magneto-energy spectrum can be written as

$$\frac{\hbar^2 k_z^2}{2m_i^*} + (n + \frac{1}{2})\hbar\omega_{0i} = EG(E, E_{gi}, \Delta_i), \tag{7}$$

$$\omega_{0i} = \frac{eB}{m_i^*}.$$

Therefore, the electron concentration takes the form

$$n_0 = \frac{eBg_v\sqrt{2m_i^*}}{\pi^2\hbar^2}\sum_{n=0}^{n_{max}}[\tau_1(n,E_F)+\tau_2(n,E_F)] \tag{8}$$

where $\tau_1(n,E_F)$ = Real part of $[E_0G(E_0,E_{gi},\Delta_i)-(n+\frac{1}{2})\hbar\omega_{0i}]^{1/2}$ and

$$\tau_2(n,E_F)=\sum_{r=1}^{S}Z_r[\tau_1(n,E_F)].$$

Using Eqs. (8) and (5) the magneto DMR can be written as

$$\frac{D}{\mu}=\frac{1}{e}\frac{\sum_{n=0}^{n_{max}}[\tau_1(n,E_F)+\tau_2(n,E_F)]}{\sum_{n=0}^{n_{max}}[\tau_1'(n,E_F)+\tau_2'(n,E_F)]}. \tag{9}$$

For $\Delta_i\to\infty$, as for the two-band Kane model, Eq. (7) assumes the well-known form [19]

$$E(1+E\alpha_i)=\frac{\hbar^2k_z^2}{2m_i^*}+(n+\frac{1}{2})\hbar\omega_{0i}. \tag{10}$$

The basic forms for the electron concentration and the magneto DMR as given by Eqs. (8) and (9) for the three-band Kane model will be unaltered for the two-band Kane model where

$$\tau_1(n,E_F)=\text{Real part of }[E_0(1+E_0\alpha_i)-(n+\frac{1}{2})\hbar\omega_{0i}]^{1/2}.$$

In the absence of broadening, together with condition $\alpha_i\cdot E_F\ll 1$, the expressions for the electron concentration and the magneto DMR for the two-band Kane model can, respectively, be expressed as

$$n_j=N_c\theta_0\sum_{n=0}^{n_{max}}\left[\left\{(1+\frac{3}{2}\alpha_ib)F_{-1/2}(\eta')+\frac{3}{4}\alpha_ik_BTF_{1/2}(\eta')\right\}(\overline{a})^{-1/2}\right] \tag{11}$$

and

$$\frac{D}{\mu}=\frac{k_BT}{e}\frac{\sum_{n=0}^{n_{max}}\left[\left\{(1+\frac{3}{2}\alpha_ib)F_{-1/2}(\eta')+\frac{3}{4}\alpha_ik_BTF_{1/2}(\eta')\right\}(\overline{a})^{-1/2}\right]}{\sum_{n=0}^{n_{max}}\left[\left\{(1+\frac{3}{2}\alpha_ib)F_{-3/2}(\eta')+\frac{3}{4}\alpha_ik_BTF_{-1/2}(\eta')\right\}(\overline{a})^{-1/2}\right]} \tag{12}$$

where $N_c = 2(2\pi m_i^* k_B T/h^2)^{3/2} \cdot g_v$, $\theta_0 = \hbar\omega_{0i}/k_B T$, $\bar{b} = (n + 1/2)\hbar\omega_{0i}/\bar{a}$, $\bar{a} = (1+\alpha_i(n+1/2)\hbar\omega_{0i})$, $\eta^{'} = (E_F - \bar{b})/(k_B T)$ and $F_j(\eta^{'})$ is the one parameter Fermi-Dirac integral of order j as defined in Ref. 27.

Under the condition $\alpha_i \to 0$, as for the relatively wide-band gap semiconductors, Eqs. (11) and (12) get simplified to the forms as given in Ref. 24.

2.2. Formulation of magneto DMR in II-VI SL's with graded interface and the constituent materials

The energy spectra of the conduction electrons of the bulk specimens of the constituent materials of II-VI SL's are given by [25,28]

$$E = \frac{\hbar^2 k_\perp^2}{2m^*_{\perp,1}} + \frac{\hbar^2 k_z^2}{2m^*_{||,1}} + \overline{\lambda} k_\perp \tag{13}$$

and

$$\frac{\hbar^2 k^2}{2m_2^*} = EG(E, E_{g2}, \Delta_2) \tag{14}$$

where $m^*_{\perp,1}$ and $m^*_{||,1}$ are the transverse and the longitudinal band edge effective masses of the electrons of the material 1, $\overline{\lambda} = \pm C_0$ where C_0 represents the splitting of the two-spin states by spin-orbit coupling and the crystalline field. All the notations of Eq. (14) have already been defined in connection with Section 2.1. The expressions for electron concentration and magneto DMR in II-VI SL are given by

$$n_0 = \frac{eBg_v}{2\pi^2\hbar l_0} \sum_{n=0}^{n_{max}} [Q_1(n, E_F) + Q_2(n, E_F)] \tag{15}$$

and Eq. (6) where

$$K^{'}(E,n) = \left[\frac{2m^*_{||,\perp}}{\hbar^2}\left\{E_F - \frac{\hbar eB}{m^*_{1,\perp}}\left(n+\frac{1}{2}\right) - \overline{\lambda}\left\{\frac{2eB}{\hbar}\left(n+\frac{1}{2}\right)\right\}^{1/2}\right\}\right]^{1/2}. \tag{16}$$

We shall now derive an expression of the electron concentration and magneto DMR by using Eq. (13). Under a quantizing magnetic field B along z-direction, the electron energy spectrum assumes the form

$$E = \frac{\hbar^2 k_z^2}{2m^*_{||,1}} + \frac{\hbar eB}{m^*_{\perp,1}}\left(n+\frac{1}{2}\right) + \overline{\lambda}\left[\left(n+\frac{1}{2}\right)\frac{2eB}{\hbar}\right]^{1/2}. \tag{17}$$

The electron concentration and DMR assume the forms

$$n_0 = \frac{eBg_v\sqrt{2m^*_{1,||}}}{2\pi^2\hbar^2}\sum_{n=0}^{n_{max}}[\tau_1(n,E_F)+\tau_2(n,E_F)] \tag{18}$$

and Eq. (9) where

$$\tau_1(n,E_F) = \text{Real part of } \left[E_0 - \frac{\hbar eB}{m^*_{\perp,1}}\left(n+\frac{1}{2}\right) - \overline{\lambda}\left[\left(n+\frac{1}{2}\right)\frac{2eB}{\hbar}\right]^{1/2}\right]^{1/2}. \tag{19}$$

For $\overline{\lambda} \to 0$, $m^*_{||,1} = m^*_{\perp,1} = m^*_1$ and neglecting broadening, Eqs. (18) and (19) assume the well-know forms for parabolic energy bands as given in Ref. 24.

2.3. Formulation of magneto DMR in PbSnTe/PbTe SL's with graded interface and the constituent materials

The $E - \vec{k}$ relation of the bulk specimens of the constituent materials of PbSnTe/PbTe SL can be expressed by [29]

$$E = \frac{\hbar^2 k_\perp^2}{2m^{*,-}_{i,\perp}} + \frac{\hbar^2 k_z^2}{2m^{*,-}_{i,||}} +$$

$$+\left[P_{\perp,i}k_\perp^2 + P^2_{||,i}k_z^2 + \left(\frac{\hbar^2k_\perp^2}{2m^{*,+}_{\perp,i}} + \frac{E_{gi}}{2} + \frac{\hbar^2k_z^2}{2m^{*,+}_{||,i}}\right)^2\right]^{1/2} - \frac{E_{gi}}{2}, \quad i=1,2. \tag{20}$$

$m^{*,+,-}_\perp$ and $m^{*,+,-}_{||}$ represent the contributions to the transverse and longitudinal band-edge effective masses arising from the $\vec{k}\cdot\vec{p}$ perturbation with other bands taken to the second order, and $P_\perp$ and $P_{||}$ represent momentum-matrix elements in the transverse and longitudinal directions, respectively. In this cases the basic forms of Eqs. (4) and (6) remain unchanged. The function $K^{'}(E,n)$ is defined in Appendix A2. For bulk specimens, the electron concentration and the magneto DMR assume the forms

$$n_0 = \frac{eBg_v}{\pi^2\hbar}\sum_{n=0}^{n_{max}}[\tau_1(n,E_F)+\tau_2(n,E_F)] \tag{21}$$

and Eq. (9) where

$$\tau_1(n, E_F) = \text{Real part of } \left[\overline{\alpha_i} E_0 + C_i - \sqrt{\gamma_i E_0^2 + g_i E_0 + H_i}\right]^{1/2} \tag{22a}$$

and

$$\tau_2(n, E_F) = \sum_{r=1}^{s} Z_r[\tau_1(n, E_F)]$$

and the other notations are defined in Appendix A2.

Under the conditions $m^{*+,-}_{||,\perp} \to \infty$ and $p^2_{||} = p^2_{\perp} = \hbar^2 E_g/2m^*_i$, Eq. (20) assumes the form

$$E(1 + \alpha_i E) = \frac{\hbar^2 k^2}{2m^*_i} \tag{22b}$$

the well-known result of the two-band model of Kane [19].

2.4. Formulation of magneto DMR for strained layers SL with graded interface and constituting materials

The dispersion relation of conduction electrons in bulk specimens of the strained small-gap materials can be written, following Ref. 30, as

$$\left(\frac{k_x}{a^*(E)}\right)^2 + \left(\frac{k_y}{b^*(E)}\right)^2 + \left(\frac{k_z}{c^*(E)}\right)^2 = 1 \tag{23}$$

where the notations have been defined in Ref. 30.

In this case the forms of Eqs. (4) and (6) will be unaltered where

$$K^{'}(E, n) = \left[(E + S^z_1)^{-1}(3E^2 + Eq_1 - R_1)(E + T_1) - (n + \frac{1}{2})\hbar\omega_1(E)\right]^{1/2},$$

$$S^z_i = E_{gi} - C^c_i \epsilon_i - (a_{0i} + C^c_i)\epsilon_i + 3b_{0i}\epsilon_{zzi} - b_{0i}\epsilon_i,$$

C^c_i is the conduction band deformation potential constant,

$$\epsilon_i = \epsilon_{xxi} + \epsilon_{yyi} + \epsilon_{zzi},$$

$$a_{0i} = -\frac{l_i + 2m_i}{3},$$

$$b_{0i} = \frac{l_i - m_i}{3},$$

$$d_{0i} = \frac{2n_i}{\sqrt{3}},$$

l_i, m_i and n_i are the matrix elements of the strain projection operator,

$$q_i = \frac{3E_{gi}}{2e_i^2} - \frac{3C_i^c \epsilon_i}{e_i^2},$$

e_i is the momentum-matrix elements,

$$R_i = \frac{\zeta_i \epsilon_{xyi}^2}{e_i^2} + \frac{3}{2}\frac{C_i^c \epsilon_i}{e_i^2}(E_{gi} - \epsilon_i C_i^c),$$

ζ_i is a constant describing the strain interaction between the conduction and the valence bands,

$$T_i = E_{gi} - \epsilon_i C_i^c, \quad \omega_1(E) = \frac{eB}{M_1(E)},$$

$$M_1(E) = \frac{\hbar^2}{2} \cdot (E + S_1^z)\left[\left(E + S_1^x - \frac{1}{2}\chi_1\right)\left(E + S_1^x + \frac{1}{2}\chi_1\right)\right]^{-1/2},$$

$$\chi_i = \sqrt{3} d_{0i} \epsilon_{xyi},$$

$$S_i^x == E_{gi} - \epsilon_i C_i^c + 3b_{0i}\epsilon_{xxi} - b_{0i}\epsilon_i - (a_{0i} + C_i^c)\epsilon_i,$$

$$K_0(E,n) = \left[(E_1 + S_2^z)^{-1}(3E_1^2 + E_1 q_2 - R_2)(V_0 - E - T_2) + (n + \frac{1}{2})\hbar\omega_2(E_1)\right]^{1/2},$$

$$E_1 = E - V_0, \quad \omega_2(E_1) = \frac{eB}{M_2(E_1)},$$

$$M_2(E_1) = \frac{\hbar^2}{2} \cdot (E_1 + S_2^z) \left[\left(E_1 + S_2^x - \frac{1}{2}\chi_2 \right) \left(E_1 + S_2^x + \frac{1}{2}\chi_2 \right) \right]^{-1/2}.$$

For bulk specimens the basic forms of Eqs. (21) and (22a) will not change where

$$\tau_1(n, E_F) = \text{Real part of } \left[f_i^*(E_0) \left\{ 1 - (n + \frac{1}{2}) \frac{2eB}{\hbar} \{ a_i^*(E_0) b_i^*(E_0) \}^{-1} \right\}^{1/2} \right], \tag{24}$$

$$f_i^*(E_0) = \sqrt{\frac{L_i(E_0)}{C_i^*(E_0)}}$$

and

$$L_i(E_0) = 3E_0^2 + E_0 q_i - R_i.$$

In the absence of stress and under the substitution $e_i^2 = 3\hbar^2(E_{gi}/4m_i^*)$, Eq. (23) assumes the same form as given by Eq. (22b).

2.5. Formulation of magneto DMR in HgTe/CdTe SL with graded interface and the constituent materials

The dispersion relation of the conduction electrons of constituent materials of HgTe/CdTe can, respectively, be expressed [31,25] as

$$E = \frac{\hbar^2 k^2}{2m_1^*} + \frac{3e^2 k}{128\epsilon_s} \tag{25}$$

and

$$\frac{\hbar^2 k^2}{2m_2^*} = EG(E, E_{g2}, \Delta_2) \tag{26}$$

where ϵ_s is the permittivity of HgTe. In this case the basic forms of Eqs. (4) and (6) remain unchanged where

$$K_0(E_n) = \left[2m_2^* \hbar^{-2} E^{'} G(E - V_0, \alpha_2, \Delta_2) + \frac{2eB}{\hbar}(n + \frac{1}{2})\right]^{1/2}$$

and

$$K^{'}(E,n) = \left[(m_1^*)^2 \hbar^{-4} \left\{-\frac{3e^2}{128\epsilon_s} + \sqrt{\left(\frac{3e^2}{128\epsilon_s}\right)^2 + \frac{2E_0\hbar^2}{m_1^*}}\right\}^2 - \frac{2eB}{\hbar}(n + \frac{1}{2})\right]^{1/2} .$$

The electron concentration and the magneto DMR for HgTe assume the same form as Eqs. (21) and (22a) where

$$\tau_1(n, E_F) = \text{Real part of } [K^{'}(E_0, n)].$$

Under the condition $\epsilon_s \to \infty$, Eq. (25) assumes the form $E = \hbar^2 k^2 / 2m_1^*$ which is the well-known equation for parabolic energy bands.

3. Suggestion for determining the DMR in degenerate semiconductors having arbitrary dispersion law

The thermoelectric power of electrons under magnetic quantization can be expressed by [32]

$$Z = \frac{V}{en_0} \tag{27}$$

where V is the magneto-entropy per unit volume. From Eq. (27) we get

$$Z = \frac{\pi^2 k_B^2 T}{3en_0} \left(\frac{\partial n_0}{\partial E_F}\right) . \tag{28}$$

Combining Eqs. (5) and (28) we get

$$\frac{D}{\mu} = \frac{\pi^2 k_B^2 T}{3Ze^2}. \tag{29}$$

Therefore, we can determine D/μ from Z for degenerate materials having arbitrary dispersion laws.

We can summarize the mathematical background in the following way. The energy band spectra of III-V, II-VI, PbTe/PbSnTe, strained semiconductors and HgTe are described by the Kane [15,25], Hopfield [28], Dimmock [29], Seiler [30] and Yakovlev [31] models. We have formulated the expressions of DMR's under magnetic quantization in III-V, II-VI, PbTe/PbSnTe, strained layer and HgTe/CdTe SL's with graded interfaces and that of the constituent materials without any approximations of band parameters. We have shown that under certain limiting conditions, Kane, Hopfield, Dimmock, Seiler and Yakovlev models reduce to the results of parabolic model as shown in Ref. 24. The above statement is the indirect theoretical test of our analysis. Besides, we have suggested the experimental method of determining the Einstein relation in degenerate materials having arbitrary dispersion laws.

4. *Results and discussion*

Using Eqs. (4), (6) and taking the parameters of GaAs/Ga$_{1-x}$Al$_x$As SL from Table 1 together with $V_0 = 0.3228$ eV, $\Delta_0 = 0.5$ nm, $l_0 = 12$ nm, $a_0 = 5$ nm, $T_D = 7.3$ K and $B = 2$ T, we have plotted the normalized magneto DMR as a function of electron concentration as shown in Fig. 1 (Curve l). In the figure the same dependence has also been plotted for the constituent materials using Eqs. (8) and (9). Using Eqs. (15) and (16) and taking the parameters of CdS/CdTe SL from Table 2 and the other common parameters as given for GaAs/Ga$_{1-x}$Al$_x$As SL, we have calculated the normalized magneto DMR as a function of n_0 in which the same dependence for the constituent materials has also been calculated by using Eqs. (18) and (19). Using the appropriate equations and taking the band parameters for PbSnTe/PbTe, InAs/GaSb and HgTe/CdTe SL's from Tables 3, 4, 5 and the other common parameters as given for GaAs/Ga$_{1-x}$Al$_x$As SL we have calculated the normalized magneto DMR's as functions of n_0 in which the same dependence for the constituent materials of the aforementioned SL's has also been calculated by using the appropriate equations for the purpose of comparison. In Fig. 2, we have plotted all the above results as a functions of $1/B$ assuming $n_0 = 10^{23}$ m^{-3}.

TABLE 1.
Band parameters of GaAs/Ga$_{1-x}$Al$_x$As *SL [33].*

GaAs	Ga$_{1-x}$Al$_x$As
$m_1^* = 0.067m_0$	$m_2^* = m_1^* + \Theta m_0$, $\Theta = 0.083$
$E_{g1} = 1.5$ eV	$E_{g2} = (1.5/0.067)(\Theta + \frac{m_1^*}{m_0})$ eV
$\Delta_1 = 0.33$ eV	$\Delta_2 = (0.33/0.067)(\Theta + \frac{m_1^*}{m_0})$ eV

TABLE 2.
Band parameters of CdS/CdTe *SL [3].*

CdS	CdTe
$m^*_{\perp,1} = 0.7m_0$	$m_2^* = 3\hbar^2 E_{g2}/4T_6^2$
$m^*_{\|\|,1} = 0.5m_0$	$E_{g2} = (-0.304 + 5\times10^{-4}T + 0.914 - 10^{-3}T)$ eV
$\overline{\lambda} = \pm1.2\times10^{-9}$ eVm	$T_6^2 = 21\hbar^2/2m_0$, $\Delta_2 = 0.9$ eV

TABLE 3.
Band parameters of PbSnTe/PbTe *SL [7].*

PbSnTe	PbTe
$m^{*,-}_{\perp,1} = 0.063m_0$	$m^{*,-}_{\perp,2} = 0.070m_0$,
$m^{*,-}_{\|\|,1} = 0.41m_0$	$m^{*,-}_{\|\|,2} = 0.5m_0$,
$m^{*,+}_{\perp,1} = 0.089m_0$	$m^{*,+}_{\perp,2} = 0.010m_0$,
$m^{*,+}_{\|\|,1} = 1.6m_0$	$m^{*,+}_{\|\|,2} = 1.4m_0$,
$P_{\|\|,1} = 137$ meVnm	$P_{\|\|,2} = 150$ meVnm,
$P_{\perp,1} = 464$ meVnm	$P_{\perp,2} = 486$ meVnm,
$E_{g1} = 90$ meV	$E_{g2} = 190$ meV

TABLE 4.
Band parameters of InAs/GaSb *SL [33,30].*

InAs	*GaSb*
$m_1^* = 0.023m_0$, $E_{g1} = 0.041$ *eV*	$m_2^* = 0.048m_0$, $E_{g2} = 0.081$ *eV*
$e_1 = 10^{-10}$ *eVm*, $\zeta_1 = 2$ *eV*	$e_2 = 14\times10^{-11}$ *eVm*, $\zeta_2 = 4$ *eV*
$C_1^c = 20$ *eV*, $(S_{11}) = 0.69\times10^{-3}$ *(kbar)*$^{-1}$	$C_2^c = 30$ *eV*, $(S_{11})_2 = 0.6\times10^{-3}$ *(kbar)*$^{-1}$
$(S_{22})_1 = 0.8\times10^{-3}$ *(kbar)*$^{-1}$	$(S_{22})_2 = 0.42\times10^{-3}$ *(kbar)*$^{-1}$
$\sigma = 4$ *kbar*	$(S_{33})_2 = 0.39\times10^{-3}$ *(kbar)*$^{-1}$
$(S_{33})_1 = 0.3\times10^{-3}$ *(kbar)*$^{-1}$	$(S_{12})_2 = 0.5\times10^{-3}$ *(kbar)*$^{-1}$
$(S_{12})_1 = 0.48\times10^{-3}$ *(kbar)*$^{-1}$	$a_{02} = -10$ *eV*
$a_{01} = -12$ *eV*, $b_{01} = -1.8$ *eV*	$b_{02} = -2$ *eV*
$d_{01} = -4.4$ *eV*	$d_{02} = -5$ *eV*

TABLE 5.
Band parameters of HgTe/CdTe *SL [33].*

HgTe	CdTe
$m_1^* = 0.025 m_0$ $\epsilon_s = 20\epsilon_0$	The values of the band parameters are given in the Table 2.

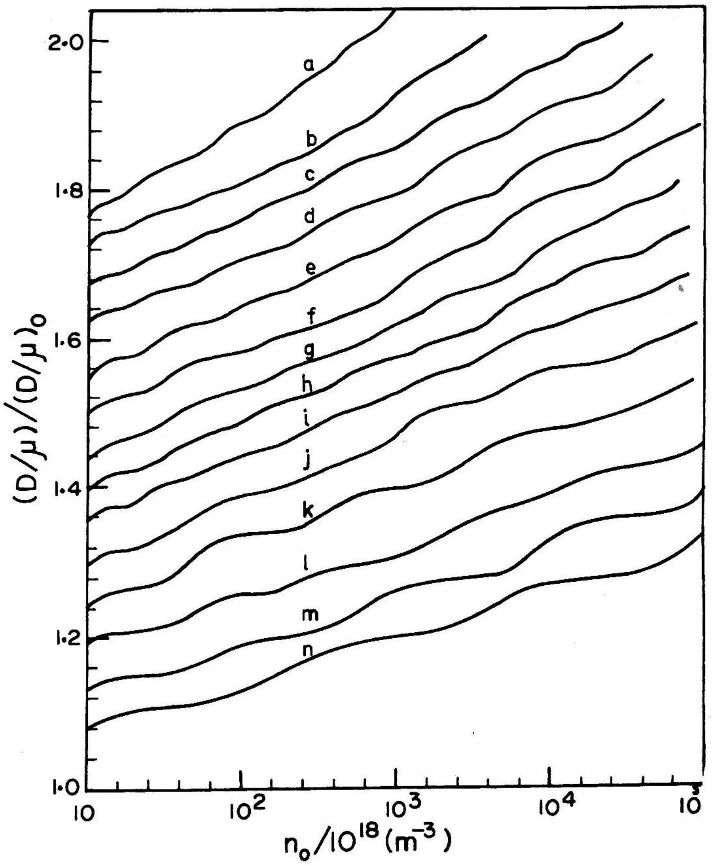

Fig. 1. Plot of the normalized DMR's as functions of electron concentration for (a) HgTe/CdTe *SL; (b) bulk* HgTe*; (c) bulk* CdTe*; (d)* CdS/CdTe *SL; (e) bulk* CdS*; (f)* PbSnTe/PbTe *SL; (g) bulk* PbSnTe*; (h) bulk* PbTe*; (i)* InAs/GaSb *SL; (j) bulk* InAs*; (k) bulk* GaSb*; (l)* $GaAs/Ga_{1-x}Al_xAs$ *SL; (m) bulk* GaAs *and (n) bulk* $Ga_{1-x}Al_xAs$.

It appears from Fig. 2 that the DMR's in SL's and constituent materials oscillate with $1/B$. The oscillatory dependence is due to the crossing of the Fermi level by the Landau subbands. It occurs in steps resulting from succesive reduction in the number of occupied Landau levels within the Fermi level. There would be a discontinuity in the density-of-states function resulting in a peak of oscillations. Under magnetic quantization, the periodicity in $1/B$ is reflected in a number of physical properties due to the profound change of the band shape of carriers. The origin of the oscillations in DMR is the same as that of the Shubnikov-de Haas oscillations. For extremely large value of the quantizing magnetic field, the condition of the quantum limits will be reached when the DMR will be found to decrease monotonically with increasing magnetic field. From Fig. 2 it also appears that the SL structure enhances the DMR in the whole range of magnetic field considered.The numerical value of the DMR is largest for HgTe/CdTe SL and least for GaAs/$Ga_{1-x}Al_x$As SL. From Fig. 1 it appears that the DMR in SL increases with increasing electron concentration in an oscillatory manner at a rate greater than for the corresponding constituent materials. It is again noted that DMR increases nonlinearly with concentration both for all SL's and for the constituent materials. The classical value of the DMR is k_BT/e and is equal to 0.36 meV at 4.2 K. This is, therefore, not shown in the figures.

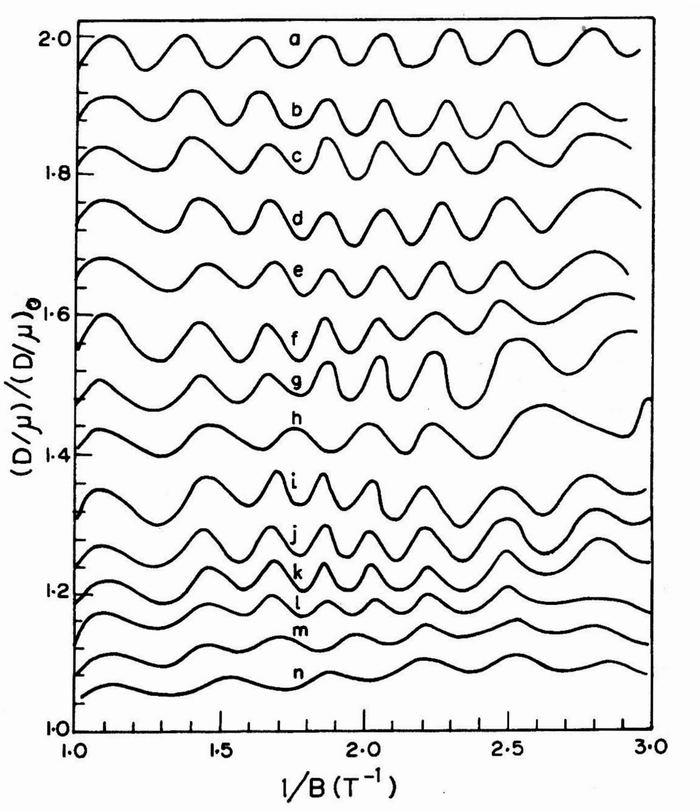

Fig. 2. Plot of normalized DMR's as a functions of $1/B$ for the cases shown in Fig. 1.

It appears from both the figures that the DMR oscillates with n_0 and $1/B$, respectively, under magnetic quantization though the nature of oscillations are different than in constituent materials. In the case of a SL, the period of oscillations is dependent also on periodic function involving the SL spacing and, consequently, the oscillatory function, being determined by different types of oscillations, is of composite character. This would further be modified in the presence of higher mini-bands. The enhanced oscillatory features of the DMR indicates that the various magneto-transport coefficients of a SL of non-parabolic semiconductors would be rather different from that of the constituent materials. These oscillatory features would also be of composite character particularly in non-parabolic SL's. Since the SL direction has a mini-band structure with alternative alowed and forbidden regions, the density-of-states function will be non zero only for such values of the electron energy for which the z-component of the energy lies within a mini-band corresponding to a given magnetic quantum number. Moreover, the density-of-states function becomes infinite at energies corresponding to both the lower and upper edges of each mini-band which is obviously a phenomenon characteristic only for a SL structure. In general, the density-of-states function is dominated from the contributions of the mini-bands. The Fermi energy in the SL is greater than that in the bulk for the same electron concentration [19]. Since the DMR is a monotonous function of Fermi energy, therefore the numerical values of the DMR in a SL is greater than that of the constituent materials. Thus in view of the aforementioned facts we can infer that the DMR in SL will be different than in the constituent materials.

We have used the three-band model of Kane [25], as the dispersion relation of the constituent materials of $GaAs/Ga_{1-x}Al_xAs$ SL. The three-band Kane model is valid for III-V compounds but should be used as such for studying the electron properties of n-InAs (in the absence of stress) where the spin-orbit splitting parameter (Δ_i) is of the order of the band gap E_{gi}. However, for many semiconductors $\Delta_i \gg E_{gi}$ (e.g. InSb). Under this condition the complicated Eq. (7) gets simplified into the form [19], $E(1+\alpha_i E) = (n+1/2)\hbar\omega_{oi} + (\hbar^2 k^2/2m_i^*)$ which is our Eq. (10). For $E_{gi} \to \infty$, as for parabolic semiconductors, the above equation assumes the well-known form

$$E = (n + \frac{1}{2})\hbar\omega_{0i} + \frac{\hbar^2 k_z^2}{2m_i^*}$$

as derived by Landau. For CdS/CdTe SL we have used the complete dispersion law for CdS as given by Eq. (13) and the three-band model of Kane for CdTe. Under certain limiting conditions, the electron energy spectrum as given by Eq. (13) converts into that of a parabolic energy band. For PbSnTe/PbTe SL we have used the Dimmock model [29] as given by Eq. (20) which is the best model for PbTe/PbSnTe type materials as stated in the literature. Under the conditions $m^{+,-}_{||,\perp} \to \infty$, the Dimmock model converts into the two–band Kane model [19]. For strained layer SL we have used the Seiler model [30] as given by Eq. (23) for the dispersion relation of the bulk materials as this is the best model for strained semiconductors. In HgTe/CdTe SL, HgTe is a gapless semiconductor whose dispersion relation is governed by Eq. (25). In formulating the SL dispersion law, we have taken into account the influence of the finite width of the interface. Thus our theoretical formulation covers various semiconductors and SL's having different band structures. We must note that the study of the transport phenomena and the formulation of the electronic properties of semiconductors and SL's are based on the dispersion relations of the electrons in such materials.

It may be noted that the DMR will, in general, be anisotropic in the presence of a quantizing magnetic field. For investigating the DMR in the presence of the magnetic field, we have to determine the element D_{zz}/μ_{zz} of the corresponding tensor. The DMR defined here refers to the direction z of the applied magnetic field.

Recently, the mobility in small gap materials and semiconductors heterostructures has been extensively investigated, but the diffusivity of such 3D electron gases much less. It must be mentioned that the diffusion constant is a very important device parameter and the accurate experimental determination of the diffusion constant is rather difficult. Therefore, our theoretical results can be used to determine the diffusivity of the electrons in SL's, even for parabolic semiconductors, both in the presence and absence of magnetic quantization, since the mobility can be experimentally determined.

It may be noted that the DMR is related to the $\mathrm{d}n_0/\mathrm{d}E_F$ as given by Eq. (5). Our suggestion for the experimental determination of the DMR for materials having arbitrary band structure, as given by Eq. (29), does not contain any band parameters. For constant temperature D/μ varies as Z^{-1}. Only the experimental values of Z for any model, as a function of electron concentration, will give the experimental values of the DMR. Since the experimental data for the thermoelectric power of the above SL's under magnetic quantization are not available in the literature to the best of our knowledge, we have no data for comparison. Since the thermoelectric power decreases with increasing electron concentration in an oscillatory manner, from Eq. (29) we can conclude that the DMR under magnetic quantization will increase with increasing electron concentration in the oscillatory fashion which is evident in Fig. 1. The above statement is the indirect theoretical test of our analysis. The experimental value of the thermoelectric power of electrons under magnetic quantization for SL's will provide an experimental check on the DMR and also a technique for probing the band structures. It may be noted that we have not considered other types of SL's or other physical variables. The variations of the DMR are totally band structure dependent. With different sets of the energy band parameters, we shall get the different numerical values of the DMR though the nature of variations will not alter. The qualitative nature of variations of the DMR's, as shown here, would be similar for other SL's. Finally, we would like to state that the basic aim of the present paper is not solely to demonstrate the effect of magnetic quantization on the DMR of the heterostructures and the constituent bulk materials, but also to suggest an experimental method determining the Einstein relation in degenerate materials having arbitrary dispersion laws.

Appendix 1.

The function $\rho(E,n)$ is defined as follows

$$\rho(E,n) = \left[\cos^{-1}\left(\frac{\psi(E,n)}{2}\right)\right]^2 \tag{A1}$$

where

$$\psi(E,n) = 2\cosh\{\beta(E,n)\}\cos\{\gamma(E,n)\} + \epsilon(E,n)\sinh\{\beta(E,n)\}\cdot$$

$$\sin\{\gamma(E,n)\} + \Delta_0\left[\left(\frac{K_0^2(E,n)}{K'(E,n)} - 3K'(E,n)\right)\cosh\{\beta(E,n)\}\cdot\right.$$

$$\left.\sin\{\gamma(E,n)\} + \left(3K_0(E,n) - \frac{CK'^2(E,n)}{K_0(E,n)}\right)\sinh\{\beta(E,n)\}\cos\{\gamma(E,n)\}\right]$$

$$+\Delta_0\left[2\left(K_0^2(E,n) - K'^2(E,n)\right)\cosh\{\beta(E,n)\}\cos\{\gamma(E,n)\}\right.$$

$$\left.+\frac{1}{12}\left(\frac{5K_0^3(E,n)}{K'(E,n)} + \frac{5K'^3(E,n)}{K_0(E,n)} - 34K'(E,n)K_0(E,n)\right)\cdot\sinh\{\beta(E,n)\}\sin\{\gamma(E,n)\}\right]$$

$$\epsilon(E,n) = \frac{K_0(E,n)}{K'(E,n)} - \frac{K'(E,n)}{K_0(E,n)}, \quad \beta(E,n) = (a_0 - \Delta_0)K_0(E,n),$$

$$K_0(E,n) = \left[\frac{2eB}{\hbar}(n+\frac{1}{2}) + 2m_2^* E'\hbar^{-2}G(E - V_0, \alpha_2, \Delta_2)\right]^{1/2},$$

$$\gamma(E,n) = K'(E,n)(b_0 - \Delta_0)$$

and

$$K'(E,n) = \left[2m_1^* E\hbar^{-2}G(E,\alpha_1,\Delta_1) - \frac{2eB}{\hbar}(n+\frac{1}{2})\right]^{1/2}.$$

Appendix 2.

The function $K^{'}(E,n)$ is defined as follows:

$$K^{'}(E,n) = \left[E\overline{\alpha_i} + C_i - (\gamma_i E^2 + E g_i + H_i)^{1/2}\right]^{1/2} \tag{A2}$$

where

$$\overline{\alpha_i} = \frac{b_i}{b_i^2 - t_i}, \quad b_i = \frac{\hbar^2}{2m^{*,-}_{||,i}},$$

$$t_i = \left(\frac{\hbar^2}{2m^{*,+}_{||,i}}\right)^2, \quad C_i = \frac{1}{2} - \beta_i, \quad \beta_i = \frac{d_i - 2a_i b_i}{2(b_i^2 - t_i)},$$

$$d_i = P^2_{||,i} + \left(\frac{\hbar^2}{2m^{*,+}_{||,i}}\right)\left[\frac{E_{gi}}{2} + \frac{\hbar eB}{m^{*,+}_{\perp,i}}(n+\frac{1}{2})\right],$$

$$\gamma_i = \frac{t_i}{(b_i^2 - t_i)^2}, \quad g_i = \delta_i + \gamma_i E_{gi},$$

$$\delta_i = \frac{b_i d_i - 2a_i t_i}{(b_i^2 - t_i)^2}, \quad a_i = \frac{\hbar eB}{m^{*,-}_{\perp,i}}(n+\frac{1}{2}),$$

$$H_i = \overline{\omega_i} + \frac{\delta_i E_{gi}}{2} + \frac{\gamma_i E_{gi}^2}{4},$$

$$\overline{\omega_i} = \frac{\gamma_i}{4t_i}\left(d_i^2 - 4a_i b_i d_i + 4G_i b_i^2 + 4t_i a_i^2 - 4t_i G_i\right),$$

$$G_i = 2eB\hbar^{-1}(n+\frac{1}{2})P^2_{\perp,i} + \left(\frac{E_{gi}}{2} + \frac{\hbar eB}{m^{*,+}_{\perp,i}}(n+\frac{1}{2})\right)^2$$

and

$$K_0(E,n) = \sqrt{\left[\gamma_2^2(E') + g_2(E') + H_2\right]^{1/2} - C_2 - E'\overline{\alpha_2}}\ .$$

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EINSTEINOVA RELACIJA U SUPERREŠETKAMA POLUVODIČA S NE-PARABOLIČNIM VRPCAMA I NEOŠTRIM MEĐUPLOHAMA KOD MAGNETSKE KVANTIZACIJE

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Razmatrana je Einsteinova relacija kod magnetske kvantizacije u superrešetkama s neoštrim međuplohama III-V i II-VI poluvodiča, PbSnTe/PbTe, HgTe/CdTe te slojeva s napetošću, te je uspoređena s onom u volumnim uzorcima gradbenih materijala. Nađeno je, uzevši GaAs/$Ga_{1-x}Al_xAs$, CdS/CdTe, PbTe/PbSnTe, InAs/GaAs i HgTe/CdTe superrešetke s neoštrim međuplohama kao primjer, da Einsteinova relacija pokazuje oscilatornu zavisnost o inverznim kvantizirajućim magnetskim poljima kao posljedica Shubnikov-de Haas efekta te raste oscilatorno s porastom koncentracije elektrona u svim slučajevima. Omjer difuzivnosti i pokretnosti je veći nego u volumnim uzorcima gradbenih materijala. Oscilacije u HgTe/CdTe superrešetkama su izrazitije nego u drugim uzorcima. Također, predložena je eksperimentalna metoda određivanja Einsteinove relacije u degeneriranim materijalima s proizvoljnim zakonom disperzije.