Multioscillation spectra of electroreflectance of germanium. Effects of band nonparabolicity

N. N. Ovsyuk and M. P. Sinyukov

Semiconductor Physics Institute, Siberian Division, USSR Academy of Sciences
(Submitted 6 April 1977; resubmitted 4 April 1978)
Zh. Eksp. Teor. Fiz. **75**, 1075–1082 (September 1978)

A high homogeneity of the electric field at the depth where the light beam is formed was attained when the electroreflectance (ER) spectra were recorded under conditions of nonuniform depletion of the space-charge region in germanium samples. Multioscillation ER spectra were obtained for transitions at the center of the Brillouin zone (orbitally degenerate critical point of the M_0 type). Assuming strict parabolicity of the heavy-hole band, these spectra were used to determine the nonparabolicity coefficients for the conduction band and for the light-hole band in the vicinity of $\mathbf{k} = 0$. It turned out that the entire ER spectrum can be described by two different parameters of the collision broadening Γ. At $T = 300$ K, for example, $\Gamma = 3$ meV for the principal signal E_0 and $\Gamma = 7$ meV for the oscillating part. It is established that the nonparabolicity of the light-hole band increases with decreasing temperature.

PACS numbers: 78.20.Dj

In accordance with the Franz–Keldysh theory,[1,2] an electroreflectance (ER) spectrum recorded under homogeneous-field conditions should have on oscillating component. These so-called Franz–Keldysh oscillations contain information on the effective masses, on the distribution of the built-in-fields, on the matrix element of the transition, and on the thermal-broadening parameter. The spatial inhomogeneity of the field in the semiconductor at the light-penetration depth can cause these oscillations from the experimental ER spectra.[3,4] To decrease the influence of the inhomogeneity, the surface field must be modulated when the spectra are recorded in a way as to deplete the space-charge region (SCR), for in that case the field decreases most slowly with increasing depth in the conductor.

To obtain "homogeneous" ER spectra at large field intensities in the SCR depletion region, Handler *et al.*[5] used doped samples. They succeeded in observing, for the first time ever, three additional oscillations in the ER spectrum of germanium to which the field was applied through an electrolyte. Comparison with the theory has shown that their experimental spectrum can be well described by using constant interband reduced masses. It is to be expected, however, that when the photon energy exceeds the interband energy at the center of the Brillouin zone by an amount of the order of the spin-orbit splitting, i.e., at $|E_g - \hbar\omega| \sim \Delta_{so}$, band-nonparabolicity effects will come into play. Handler *et al.*[5] did not succeed in obtaining a sufficiently large number of oscillations to observe these effects. In later studies,[6,7] in which the Schottky barrier was used, the conditions were likewise not optimal to obtain high homogeneity of the field. It is therefore of interest to obtain ER spectra with large numbers of oscillations, covering a wide range of photon energies, to observe the possible effects of band nonparabolicity.

It was shown in our earlier analysis[8] that when ER spectra are recorded the best field homogeneity can be obtained by obtaining nonequilibrium depletion in the SCR in samples of sufficiently high resistance.

The experimental spectra were recorded with light reflected from the (111) surface of n-Ge with donor density 1.3×10^{14} cm^{-3}, using Schottky barriers produced by sputtering a semitransparent aluminum layer. When the spectra were recorded the light was polarized in the direction of the [$\bar{1}$10] axis in the reflection plane. The resolution of the optical system, in which an MDR-2 monochromator was used, was 1 meV. To obtain the ER signal, unipolar square-wave voltage pulses were applied to the sample at a frequency 200 Hz. The spectra were registered in the region of the direction absorption edge of germanium at the orbitally degenerate point Γ for E_0 and $E_0 + \Delta_0$ transitions.

Figure 1 shows a number of ER spectra obtained at successively larger amplitudes of the surface-field modulation. It is seen that the region of the oscillations that follow the signal E_0 increases with increasing field intensity and successively distorts the spin-orbit signal $E_0 + \Delta_0$ and propagates behind it.

According to the arguments of Keldysh, Konstanti-

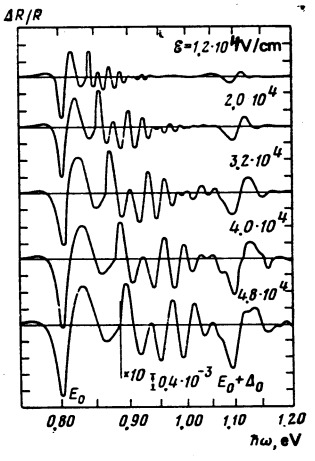

FIG. 1. ER spectra of Ge for the transitions E_0 and $E_0+\Delta_0$, plotted with increasing amplitude of the surface-field modulation. Temperature $T = 300$ K, $\mathcal{E} \parallel [111]$, light-wave polarization vector $\mathbf{e} \parallel [\bar{1}10]$. The amplitudes of the spectra, starting with the second oscillations, are magnified 10 times.

 0038-5646/78/090542-05$02.40

nov, and Perel',[9] the ER spectrum registered in an orbitally degenerate critical point is a linear combination of spectra for each individual band at this point, i.e.,

$$\frac{\Delta R}{R}(\omega, \vec{\mathscr{E}}) = \frac{A}{(\hbar\omega)^2}[BG(-\eta_l)+G(-\eta_h)], \quad (1)$$

where A is an amplitude factor that contains the square of the matrix element of the transition and the factors of the state densities in the bands, $\hbar\omega$ is the photon energy, B is the ratio of the contributions of the light- and heavy-hole bands to the ER spectrum, $G(-\eta_l)$ and $G(-\eta_h)$ are oscillating electro-optical functions for the light- and heavy-hole bands, respectively, and $\vec{\mathscr{E}}$ is the electric vector of the reflected wave.

Since the period of the oscillations is a function of the reduced mass, the oscillations from each band have different periods and their sum contains beats in certain sections of the spectrum, as can be seen in Fig. 1. The argument of the electro-optical function $G(-\eta)$ is given by

$$\eta = (E_g - \hbar\omega)/\hbar\theta, \quad (2)$$

where E_g is the energy of the critical point, $\hbar\theta = e^2\mathscr{E}^2\hbar^2/2\mu_\parallel)^{1/3}$ is the so-called electro-optical energy, and $\mu_\parallel$ is the reduced mass of the electron and hole in the field direction.

Equating the total differential of the function $G(-\eta)$ to zero, we find that the shift of the function $G(-\eta)$, and consequently also of the ER spectrum, along the energy axis, following a small change of μ by an amount $\Delta\mu$, can be expressed in the form

$$\Delta(\hbar\omega) \sim -\frac{\Delta\mu}{\mu}|\hbar\omega - E_g|, \quad (3)$$

i.e., it will increase, at equal change of the reduced mass, in proportion to the energy distance from the critical point. Consequently the influence of the nonparabolicity effects will be felt more strongly by oscillations that are farthest from E_g.

For the sake of simplicity we confine ourselves in the analysis of the ER spectra to the energy region from E_0 to $E_0+\Delta_0$, inasmuch as at higher energies a third, spin-orbit split band will contribute to the interference of the oscillations from the light- and heavy-hole bands.

In the comparison of the signal E_0 with experiment we shall use relation (1), and in the comparison of the oscillating part of the spectrum we shall replace the electro-optical functions with the asymptotic expressions obtained in Ref. 10:

$$\frac{\Delta R}{R}(\omega, \vec{\mathscr{E}})\Big|_{l,h} \sim (\hbar\omega)^{-2}(\hbar\omega - E_g)^{-1}\exp\left[-\frac{2(\hbar\omega - E_g)^{3/2}\Gamma}{(\hbar\theta_{l,h})^{3/2}}\right] \times\cos\left[\varphi + \frac{4}{3}\left(\frac{\hbar\omega - E_g}{\hbar\theta_{l,h}}\right)^{3/2}\right], \quad (4)$$

where Γ is the collision-broadening parameter, and φ is a phase shift that depends on the electron-hole interaction force and varies little with energy. This expression was chosen because it was generalized in Ref. 10 to include the case of nonparabolic bands.

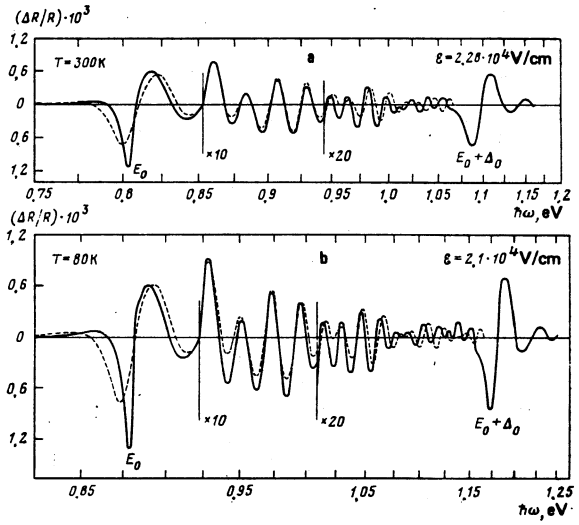

FIG. 2. Solid lines—ER spectra of Ge at 300 (a) and 80 K (b) for the transitions E_0 and $E_0+\Delta_0$. Vector $\vec{\mathscr{E}} \parallel [111]$, light-wave polarization vector $\mathbf{e} \parallel [\bar{1}10]$. Dashed lines—theoretical ER specta obtained using constant reduced masses $\mu_l = 0.0196\, m_0$ and $\mu_h = 0.0354\, m_0$. The energies are $E_g = 0.799$ and $E_g = 0.872$ eV at 300 K and 80 K, respectively. The thermal expansion parameters at both temperatures were equal to 7 meV.

Figure 2 shows the spectra obtained at 300 and 80 K, with the theoretical spectra shown dashed. To construct these spectra it was necessary to measure accurately the field intensity, to choose the effective carrier masses for a given direction of the electric field relative to the crystal axes, the value of the collision broadening, and the ratio of the contributions of the light and heavy holes to the ER spectrum.

The effective masses were calculated from the expressions[7]

$$m_0/m^*_{l,h} = -\gamma_1 - 2g(\mathbf{e}), \quad (5)$$

$$g(\mathbf{e}) = \pm[\gamma_2^2 \pm 3(\gamma_3^2 - \gamma_2^2)(e_x^2 e_y^2 + e_y^2 e_z^2 + e_z^2 e_x^2)]^{1/2}, \quad (6)$$

where m_0 is the mass of the free electron, $m^*_{l,h}$ are the effective masses of the light and heavy holes, γ_1, γ_2, and γ_3 are the Luttinger parameters, $\mathbf{e}$ is a unit vector along the electric-field direction, and $g(\mathbf{e})$ is a function of the angles the field makes with the crystal axes; the + and − signs in (6) refer to the light and heavy holes, respectively. In our case $\vec{\mathscr{E}} \parallel [111]$ and the reduced masses of the light and heavy holes are $\mu_l = 0.0196 m_0$ and $\mu_h = 0.0354 m_0$, respectively. The amplitude of the theoretical curve was chosen equal to the amplitude of the positive part of the first oscillation of the experimental spectrum.

The surface field, which determines the oscillation period, must be determined with high accuracy, higher than obtained with measurements of the volt-farad characteristics of the Schottky barrier. The field was therefore varied by 5–8% of the experimental value in order to make the theoretically obtained spectrum agree with the experimental one in the region of the first four oscillations. It was observed then that the negative maxima of E_0 of the theoretical and experimental spectra differed by as much as 4 meV, possibly as a result of Coulomb interaction or orbital degenera-

cy, effects which we did not take into account.

Until an oscillating part could be obtained in the ER spectra, it was assumed that the failure was due to the large thermal broadening. The broadening Γ for a direct transition E_0 in Ge was assumed equal to 30 meV.[11] Handler *et al.*,[5] by obtaining additional oscillations, demonstrated by the same token that Γ should be much less than 30 meV. To fit the shape and width of the peak E_0 (within the framework of the one-electron approximation), they used a value 3 meV. But then the experimentally obtained oscillation amplitude decreased with energy much faster than for the theoretically obtained oscillations, i.e., this value of the broadening did not describe the oscillating part of the spectrum.

The determination of the broadening parameter Γ from the damping of the oscillating part of a spectrum with a large number of oscillations makes it possible to measure the dependence of the broadening on the energy in a broad spectral interval. The best agreement between the oscillating parts of the theoretical and experimental spectra was obtained for both temperatures at $\Gamma = 7 \pm 0.5$ meV (as against 3 meV for the main signal E_0 at 300 K). Attention is called to two facts: first, the amplitude of the damped oscillations is described, up to the signal $E_0 + \Delta_0$, by a constant energy-independent quantity Γ; second, the broadening for the oscillating part of the spectrum remains unchanged when the temperature is lowered to 80 K, although the broadening for the signal E_0 decreases by a factor 1.5.

These experimental data demonstrate that the value of the broadening parameter Γ increases with energy near the direct edge E_0 after which it saturates and has a weak temperature dependence.

The ratio B of the contributions of the light- and heavy-hole bands to the ER spectrum was determined with the aid of the relations given by Aspnes.[7] At $\vec{\mathscr{E}} \| [111]$ and with the light wave polarized in the $[\bar{1}10]$ direction we obtain

$$\frac{\Delta R}{R}(\omega, \vec{\mathscr{E}}) \Big|_{[\bar{1}10]} = 0{,}167 D_l P_{cv}^2 G(-\eta_l) + 0{,}5 D_h P_{cv}^2 G(-\eta_h), \tag{7}$$

where D_l and D_h are the state-density factors in the bands of the light and heavy holes, respectively; P_{cv} is the interband-transition matrix element.

If it is assumed that the state-density factors are proportional to $\mu^{4/3}$ (Ref. 12) (for a three-dimensional critical point), then the ratio of the contributions of the light and heavy holes to the ER spectrum is 0.15. At this value of B, however, there are practically no beats in the theoretical spectrum and this spectrum differs significantly in shape from the experimental one. To choose the contribution ratio corresponding to the experimental spectrum, spectra were calculated with values of B ranging from 0.15 to 2.0. The best agreement with the form of the experimental spectra is obtained at $B = 0.5$, i.e., when the contribution of the *heavy-hole* band is double that of the light holes.

Comparison of the theory with experiment has shown that at no value of the field or of B can the oscillating parts of the theoretical and experimental curves be made to agree in the entire range of photon energies from E_0 to $E_0 + \Delta_0$ if the reduced masses of the light and heavy holes are kept constant.

Agreement between theory and experiment was obtained primarily by changing the ratio of the reduced masses of the heavy and light holes, inasmuch as the beats in the spectrum change their shape and their localization region when this ratio is varied. It is precisely the observation of three beat regions in the spectrum which made it possible to choose the exact value of this ratio, permitting in turn the resolution of the experimental spectrum into components due to the light- and heavy-hole bands. When the shapes of the beats of the experimental and theoretical spectra coincided, the mass ratio was found to range from 1.81 to 1.91 in the energy band from E_0 to $E_0 + \Delta_0$.

It turned out further that the functions $\hbar\theta_l(\hbar\omega)$ and $\hbar\theta_h(\hbar\omega)$ obtained after resolving the experimental into components corresponding to "light" and "heavy" holes contain terms quadratic in energy. This means that the expansion of the interband energy about the critical point, for the purpose of finding the nonparabolicity components, must extend to the term that includes k^6, i.e., must take the form

$$E_{cv}(\mathbf{k}) \Big|_{h,l} = E_g + \hbar^2 \mathbf{k}^2 / 2\mu_{h,l} - (C_1^{h,l} \mathbf{k}^4 + C_2^{h,l} \mathbf{k}^6), \tag{8}$$

where $C_{1,2}^l$ and $C_{1,2}^h$ are the interband nonparabolicity coefficients for transitions from the bands of the light and heavy holes, respectively, with thonparabolicity increasing with increasing k at $(C_1^{h,l} \mathbf{k}^4 + C_2^{h,l} \mathbf{k}^6) > 0$.

Following Kane's paper,[13] where the valence bands of germanium near $\mathbf{k} = 0$ were calculated by the $\mathbf{k} - \hat{\mathbf{p}}$ method, we assume the heavy-hole band to parabolic. In this case we can determine the nonparabolicity coefficients of the conduction band and of the light-hole band from the interband nonparabolicity coefficients. The interband-nonparabolicity coefficients C_1^h and C_2^h for transitions from the heavy-hole band must in this case be due entirely to the nonparabolicity of the conduction band, i.e., $C_1^h = C_{1c}$ and $C_2^h = C_{2c}$. For transitions from the light-hole band, the interband-nonparabolicity coefficients will be determined by the sum of the contributions of the conduction and light-hole bands:

$$C_1^l = C_{1c} + C_{1vl} \quad C_2^l = C_{2c} + C_{2vl}. \tag{9}$$

Knowing the coefficients C_{1c} and C_{2c} we can determine the coefficients C_{1cl} and C_{2vl} for the light-hole band.

We now write down separate expansions of the energy in powers of $\mathbf{k}$ near the center of the Brillouin zone for the conduction and valence bands:

$$\begin{aligned} E_c(\mathbf{k}) &= E_g + \hbar^2 \mathbf{k}^2 / 2m_c + C_{1c} \mathbf{k}^4 + C_{2c} \mathbf{k}^6, \\ E_{vh}(\mathbf{k}) &= -\hbar^2 \mathbf{k}^2 / 2m_h, \\ E_{vl}(\mathbf{k}) &= -\hbar^2 \mathbf{k}^2 / 2m_l - C_{1vl} \mathbf{k}^4 - C_{2vl} \mathbf{k}^6. \end{aligned} \tag{10}$$

Using the stationary phase method, as was done by Aspnes[10] for the expansion of the interband energy with one nonparabolicity coefficient, we have obtained an asymptotic expression for the oscillating parts of the ER spectrum, with allowance for the two nonparabolicity coefficients $C_1^{h,l}$ and $C_2^{h,l}$, in the form

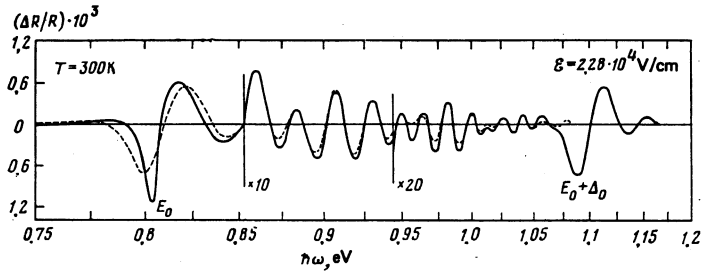

FIG. 3. Solid curve—ER spectrum at 300 K shown in Fig. 2a. Dashed curve—theoretical ER spectrum obtained using the interband nonparabolicity coefficients of (12), $\Gamma = 7$ meV, and $E_g = 0.799$ eV.

$$\frac{\Delta R}{R}(\omega, \vec{\mathscr{E}}) \sim \frac{1}{(\hbar\omega)^2(\hbar\omega - E_g)} \exp\left\{ -\frac{2(\hbar\omega - E_g)^{3/2}\Gamma}{(\hbar\theta)^{3/2}} + \frac{4C_1\mu^2\Gamma}{\hbar^4}\left(\frac{\hbar\omega - E_g}{\hbar\theta}\right)^{3/2} + \frac{8C_2\mu^3\Gamma}{\hbar^6}\frac{(\hbar\omega - E_g)^{5/2}}{(\hbar\theta)^{3/2}} - \frac{28C_1^2\mu^4\Gamma}{\hbar^8}\frac{(\hbar\omega - E_g)^{5/2}}{(\hbar\theta)^{3/2}} \right\}$$
$$\times \cos\left\{ \varphi + \frac{4}{3}\left(\frac{\hbar\omega - E_g}{\hbar\theta}\right)^{3/2} \left[1 - \frac{6}{5}\frac{C_1\mu^2}{\hbar^4}(\hbar\omega - E_g) - \frac{12}{7}\frac{C_2\mu^3}{\hbar^6}(\hbar\omega - E_g)^2 + 6\frac{C_1^2\mu^4}{\hbar^8}(\hbar\omega - E_g)^2 \right] \right\}. \quad (11)$$

From a comparison of expressions (11) and (4) it is seen that the nonparabolicity effects lead both to additional damping of the oscillations and to an energy shift of the oscillation. Aspnes,[10] for example, proposes to determine the nonparabolicity from the additional damping. But since the nonparabolicity effects influence more strongly the oscillations that are far from E_g and have low amplitude, the oscillations will vary within the limits of the experimental error, whereas the spectrum shift corresponding to this variation can be equal to the oscillation period and can be easily observed. Therefore, even though the corrections that must be introduced in the amplitude and in the period of the oscillations to account for the nonparabolicity are of the same order, the experimental conditions are such that the nonparabilicity is determined more accurately from the change of the period of the oscillations.

A comparison of the theoretical spectrum obtained with the aid of the sum of expressions (11) for transitions from the light- and heavy-hole bands with the experimental data is shown in Fig. 3. Agreement between theory and experiment was obtained when the interband nonparabolicity coefficients were

$$C_1^h = (0{,}4 \pm 0{,}1) \cdot 10^{-28}\,\text{eV} \cdot \text{cm}^4, \quad C_2^h = (-6{,}0 \pm 0{,}2) \cdot 10^{-42}\,\text{eV} \cdot \text{cm}^6,$$
$$C_1^l = (1{,}2 \pm 0{,}3) \cdot 10^{-28}\,\text{eV} \cdot \text{cm}^4, \quad C_2^l = (-24{,}6 \pm 0{,}3) \cdot 10^{-42}\,\text{eV} \cdot \text{cm}^6. \quad (12)$$

This yields the nonparabolicity coeffients for the conduction and light-hole bands

$$C_{1c} = (0{,}4 \pm 0{,}1) \cdot 10^{-28}\,\text{eV} \cdot \text{cm}^4, \quad C_{2c} = (-6{,}0 \pm 0{,}2) \cdot 10^{-42}\,\text{eV} \cdot \text{cm}^6,$$
$$C_{1vl} = (0{,}8 \pm 0{,}4) \cdot 10^{-28}\,\text{eV} \cdot \text{cm}^4, \quad C_{2vl} = (-18{,}6 \pm 0{,}5) \cdot 10^{-42}\,\text{eV} \cdot \text{cm}^6. \quad (13)$$

The band structure obtained for germanium by using these coefficients is shown by the solid lines in Fig. 4, where the straight solid line in the valence band is constructed for a parabolic heavy-hole effective mass $m_h^* = 0.508 m_0$. The dashed $E(\mathbf{k}^2)$ line in the conduction band was obtained with Kane's three-band model[14] with a nonparabolicity coefficient

$$C_{1c} = -\left(\frac{\hbar^2}{2m_c}\right)^2 \left(1 - \frac{m_c}{m_0}\right)^2 \left[\frac{3E_g + 4\Delta + 2\Delta^2/E_g}{(E_g + \Delta)(3E_g + 2\Delta)}\right]. \quad (14)$$

The $E(\mathbf{k}^2)$ plot for the light-hole band, obtained in the same model, lies much higher than the experimental curve. The reason is that Kane's model neglects the interaction with bands higher than the conduction band. To compare the theory with the experiment we have therefore used for the light holes the more accurate function $E(\mathbf{k}^2)$ obtained by Kane by the $\mathbf{k} - \hat{\mathbf{p}}$ method for Ge.[13] The smaller range of the experimental values of $E(\mathbf{k}^2)$ for the light-hole band in Fig. 4 is due to the fact that the transitions from this band are localized closer to the center of the Brillouin zone than those from the heavy-hole band at the same values of the interband energy. It is seen from the figure that theory agrees well with experiment at $(\hbar\omega - E_g) \lesssim 200$ meV.

Comparison of theory with experiment at 80 K shows that the nonparabolicity of the conduction band remains the same as at room temperature, and the nonparabolicity of the light-hole band increases slightly.

In conclusion, the authors thank O. A. Makarov for help with the work and I. G. Neizvestnyĭ for a discussion of the results.

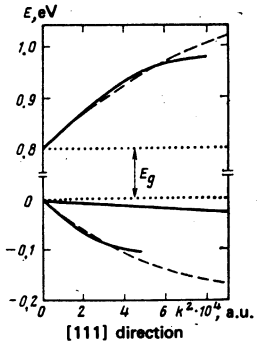

FIG. 4. Solid lines—band structure of Ge, obtained using the band nonparabolicity coefficients (13). The straight line in the valence band is drawn for a parabolic heavy-hole effective mass $m_h^* = 0.508\, m_0$. Dashed line in valence band—plot of $E(\vec{k}^2)$ for the heavy-hole band, taken from Kane's paper.[13] Dashed line in conduction band—plotted in accord with Kane's three-band model.

[1] W. Franz, Z. Naturforsch. Teil A **13**, 484 (1958).
[2] L. V. Keldysh, Zh. Eksp. Teor. Fiz. **34**, 1138 (1958) [Sov. Phys. JETP **7**, 788 (1958)].
[3] D. E. Aspnes and A. Frova, Solid State Commun. **7**, 155 (1969).

[4]V. A. Tyagai, Ukr. Fiz. Zh. 15, 1164 (1970).
[5]P. Handler, S. Jasperson, and S. Koeppen, Phys. Rev. Lett. 23, 1387 (1969).
[6]D. E. Aspnes, Phys. Rev. Lett. 31, 230 (1973).
[7]D. E. Aspnes, Phys. Rev. B 12, 2297 (1975).
[8]I. G. Neizvestnyĭ, N. N. Ovsyuk, and M. P. Sinyukov, Pis'ma Zh. Eksp. Teor. Fiz. 24, 393 (1976) [JETP Lett. 24, 359 (1976)].
[9]L. V. Keldysh, O. V. Konstantinov, and V. I. Perel', Fiz. Tekh. Poluprovodn. 3, 1042 (1969) [Sov. Phys. Semicond. 3, 876 (1970)].
[10]D. E. Aspnes, Phys. Rev. B 10, 4228 (1974).
[11]B. O. Seraphin and N. Bottka, Phys. Rev. 145, 628 (1966).
[12]D. E. Aspnes and A. Frova, Phys. Rev. B 2, 1037 (1970).
[13]E. O. Kane, J. Phys. Chem. Solids 1, 82 (1956).
[14]E. O. Kane, J. Phys. Chem. Solids 1, 249 (1957).

Translated by J. G. Adashko

Duality transformations for discrete Abelian models. Simple example of duality transformation for non-Abelian model

V. S. Dotsenko

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences
(Submitted 6 April 1978)
Zh. Eksp. Teor. Fiz. 75, 1083–1101 (September 1978)

A duality transformation is proposed for gauge and non-gauge Abelian A_N models (generalization of the Ising model, the field assumes N discrete values on a circle) to include two-, three-, and four-dimensional cubic lattice. Besides the known cases of self-duality of the Ising model (A_2 model) in two and four dimensions, an entire series of self-dual models is found (particularly the Z_3 and Z_4 self-dual models), and accordingly, the phase-transition points for them. A duality transformation is also proposed for the simple case of a discrete non-Abelian model (the symmetry group is the group of symmetry axes of the tetrahedron). The model turns out to be self-dual and accordingly the dual transformation makes it possible to find the phase-transition point.

PACS numbers: 05.50. + q

1. INTRODUCTION. DESCRIPTION OF MODELS

It is well known that the two-dimensional ($2D$) Ising model has a definite thermodynamic symmetry, as established by Kramers and Wannier.[1] The gist of this symmetry is that the partition function $Z(\beta)$, as a function of the reciprocal temperature $\beta = 1/T$, is invariant (apart from an inessential factor) to the transformation

$$\beta \to \beta^* = -\tfrac{1}{2} \ln \operatorname{th} \beta, \tag{1}$$

which converts low temperatures into high ones and vice versa. The values of $Z(\beta)$ at the points β and β^* are connected by the relation

$$Z(\beta) = (\operatorname{sh} 2\beta)^{\Omega} Z(\beta^*), \tag{2}$$

where Ω is the number of lattice points. One of the possible proofs of (2) can be found, for example, in Isihara's book.[2] The qualitative form of (1) is shown in Fig. 1. From (2) it follows that the thermodynamic properties of the high-and low-temperature phases are symmetrical.

In the reciprocal-temperature scale, there is a preferred point β_c defined by the condition $\beta^* = \beta$. From (1) we have

$$\beta_c = \tfrac{1}{2} \ln(\sqrt{2}+1). \tag{3}$$

If we assume that there is only one phase-transition point, or, which is the same, that there are only two different phases (for the Ising model this is obvious: ordered and disordered phases), then it follows from symmetry considerations that β_c is a phase-transition point. Thus, the Kramers–Wannier (KW) symmetry[1] has made it possible to obtain the phase-transition point for the $2D$ Ising model before an exact solution has been found for the model of Ref. 3.

The partition-function transformation whereby $Z(\beta)$ is expressed in terms of $Z(\beta^*)$ is called a duality transformation. The property of the Ising model, that it goes over into itself under this transformation, is called self-duality. The initial derivation of (2) was based on comparison of Van der Warden graphs of the expansions of the partition functions of the initial and dual models.[1] The KW symmetry (self-duality) is actively used in investigations of the Ising model.[4,5] Kadanoff and Ceva[5] investigated the physical meaning of the duality transformation, introduced the concept of the disorder parameter, and established that the

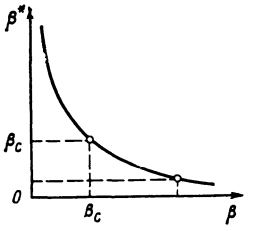

FIG. 1. Schematic plot of the function $\beta^* = -(1/2)\ln \tanh \beta$.

 0038-5646/78/090546-10$02.40