

Rashba's method of invariants

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This brief review is dedicated to the memory of E. I. Rashba and presents both a history of the development of the invariants method as applied to constructing the Hamiltonian of the effective mass method in semiconductor physics, as well as its modern use for describing a wide range of problems in two-dimensional crystals and crystals with complex magnetic and electric order.

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I. HISTORICAL REVIEW

Rashba started working in Kyiv in the Institute of Semiconductor Physics in 1954. It was the time of rapid development of semiconductor technologies and, accordingly, the development of the theory of semiconductor physics. Among many problems which Rashba dealt with, there is the method of invariants, as applied to the problem of constructing the Hamiltonian of the effective mass method. As it is well known, in semiconductors, the concentration of carriers is low, so almost all of them are close to the extrema of the energy zones, which makes it possible to greatly simplify equations of electron motion in the presence of smooth external fields (i.e. field space variations of which on the scale of the lattice constant are relatively small). This simplification is just called the effective mass method (MEM). For a simple zone, the concept of effective electron mass in a crystal was introduced back in 1946 by Pekar [1], and for a degenerate zone, the approach developed by Luttinger and Kohn in 1955 [2] became the most widespread. The effective mass method reduces the action of the crystal potential on an electron to the introduction of a certain effective mass (different from the mass of a free electron), and it is this mass that must appear in the equations of motion of an electron in smooth external fields. For a degenerate zone with n -fold degeneracy, this method allows us to present the Hamiltonian near the extremum point k_o of the zone as a matrix of dimension $n \times n$ with the inverse effective mass tensor and the effective magnetic moment tensor. The form of the matrix is determined by the symmetry of the energy zone at the extremum point k_o . In their work, Luttinger and Kohn considered an important group of semiconductor crystals, namely crystals with diamond structure, such as Si and Ge. In such crystals, the valence zone extremum is located

in the center of the Brillouin zone at the point $k_o = 0$, where the zone is threefold degenerate without taking into account the spin-orbit (SO) interaction. While obtaining the form of the Hamiltonian matrix, the authors relied on the symmetry properties of such crystals and used the general form of the basis functions of the irreducible representation T_1 of the point group O_h (we use the notations of Ref. [3] here) which transforms the state at the point $k_o = 0$.

Shortly after the publication of Ref. [2], Luttinger published a new paper [3], in which he rewrote the obtained Hamiltonian using the components I_α ($\alpha = x, y, z$) of the momentum matrix $I = 1$. To this end, he constructed combinations of the I_α matrices and their products $I_\alpha I_\beta$, analogous to the basis functions $x_\alpha x_\beta$ of the irreducible representations of the group O_h comprised in the direct product $T_1^* \times T_1$ by which the square of the wave function is transformed. This allowed Luttinger to represent the 3×3 matrix of the MEM Hamiltonian (obtained in Ref. [2]) in a compact and elegant form:

$$\begin{aligned} \hat{H} = & \alpha_1 k^2 + \alpha_2 (k_x^2 I_x^2 + k_y^2 I_y^2 + k_z^2 I_z^2) \\ & + \alpha_3 (\{k_x k_y\} \{I_x I_y\} + \{k_x k_z\} \{I_x I_z\} + \{k_y k_z\} \{I_y I_z\}) \\ & + \alpha_4 (I_x H_x + I_y H_y + I_z H_z), \end{aligned} \quad (1)$$

where $\{\}$ denotes the symmetrized product, $k_\alpha = -i\partial/\partial x_\alpha$ denotes the momentum operator, and H_α denotes the components of the external magnetic field. In this case, the form of the Hamiltonian is determined only by the symmetry properties of the crystal, and the unknown constants α_i are determined from experiment.

Luttinger's work [3] was the first illustration that the MEM matrix Hamiltonian can be presented in a compact form from the general idea of Hamiltonian invariance with respect to all symmetry transformations of the wave vector symmetry group G_{k_o} at the zone extremum. This work served as an impetus for the development of the invariant method, the rigorous exposition and development of which required several more years and a great deal of work, which was started in the works of Rashba and Sheka, and then developed and completed in detail in the works of Bir and Pikus and set forth in their fundamental book *Symmetry and Strain-Induced Effects in Semiconductors* [4], which for many years remained the only

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book where this method was detailed and shown in application. The idea behind the invariant method is that each state of the carrier near the zone extremum point k_o corresponds to some irreducible representation T_i of the wave vector symmetry group G_{k_o} . In group theory the property of irreducible representations is proved, according to which the direct product of two identical irreducible representations $T_i^* \times T_i$ of a group always possesses a unit representation, which means that from the products of the basis functions f_i and F_i of an irreducible representation T_i one can construct the invariant combination

$$I_T = \sum_i f_i^* F_i, \quad (2)$$

which does not change under all symmetry transformations of the group G_{k_o} . Similarly to the construction of the basis functions of irreducible representations F_i , we can construct basis matrices A_i of the same irreducible representations, which under the action of the group symmetry operations are transformed similarly to the basis functions. If, instead of the basis functions f_i^* , we take linear and quadratic combinations of operators $f_i^* \rightarrow \{k_\alpha, \{k_\alpha k_\beta\}, H_\alpha, \dots\}$, and, instead of the basis functions F_i , we take basis matrices of the same irreducible representations $F_i \rightarrow A_i$, then we can construct invariants I_T written through operators and matrices, from which the Hamiltonian will consist. The representations T_i the invariants of which are included in the Hamiltonian are determined by the representation by which the square of the wave function is transformed and by the representations by which the operators are transformed; it is important to take into account the symmetry of the Hamiltonian with respect to the time inversion symmetry.

In the 1950s, while working at the Institute of Semiconductor Physics in Lashkaryov's department, Rashba studied the problem of photoconductivity kinetics in hexagonal crystals A_2B_6 of the type CdS and CdSe, which is why he faced the question of the zone structure of such crystals, which are called crystals with wurtzite structure. As Rashba described in his memoirs [5], it became clear at that time that theoretical physics in Kyiv lagged far behind the cutting edge of science in this field abroad. The aforementioned works in *Physical Review* were not understood because they made extensive use of group theory. Thus, Kyiv theorists faced a serious challenge: to master the application of group theory methods to solid-state physics. To this end, special seminars were held at the institute under the guidance of Rashba with the participation of mathematicians. These seminars examined the works of Bouckaert *et al.* [6], Elliott [7], Dresselhaus [8], and others. In the paper [8], properties of SO coupling in zinc-blende crystals were considered. It was obtained that, due to the absence of inversion symmetry in such crystals, the presence of cubic in the wave vector k terms in the Hamiltonian at the center of the Brillouin zone leads to the removal of spin degeneracy in the conduction band without an external magnetic field in all directions except [100], [111], and their equivalents:

$$E_D = ak^2 \pm b\sqrt{k_x^2(k_z^2 - k_y^2)^2 + k_z^2(k_y^2 - k_x^2)^2 + k_y^2(k_x^2 - k_z^2)^2}. \quad (3)$$

This kind of spin splitting is now called Dresselhaus SO splitting. As a result of studying the group theory in 1959 and 1960, works by Rashba [9] and by Rashba and his graduate student Sheka [10] appeared, in which a detailed symmetry analysis of the energy zone structure of another important group of semiconductor crystals without an inversion center, namely crystals with a wurtzite structure, was performed, both with and without spin-orbital interaction. The main difference between these crystals and cubic crystals with a diamond and zinc-blende structure was that they have symmetry axis C_6 that makes x , y , and z axes nonequivalent. In works [9,10], irreducible representations of wave vector groups were constructed and Hamiltonians were presented for all special points of the Brillouin zone of such crystals, since at that time the positions of the zone extrema were not yet reliably known for many semiconductors. In Ref. [10], it was first shown that an extremum of the zone can exist not at a single point of the Brillouin zone, but on a circle called an *extremum loop*. For example, the dispersion law at the center of the Brillouin zone, taking into account spin-orbit interaction, has the form

$$E_R = aK_\perp^2 + bK_z^2 \pm \alpha K_\perp, \quad K_\perp = \sqrt{k_x^2 + k_y^2}. \quad (4)$$

The presence of a component that is linear in absolute value of the wave vector component lying in the plane perpendicular to the axis z leads to the fact that the extremum of the zone is realized not at a single point, but on a circle of radius $\sim |\alpha/a|$ in the plane $K_z = 0$. This type of dispersion law is now called Rashba SO coupling. Later, it turned out that the presence of spin splitting that is linear in the wave vector has a more universal character in systems without spatial inversion [11,12] and was found in a wide variety of two-dimensional (2D) structures where this spatial inversion is destroyed by the interface potential or by the electric field [13].

However, as told by Sheka, there always remained a doubt whether all terms in the Hamiltonian are taken into account. Thus, one needed a criterion allowing one to determine strictly the possible number of terms (invariants) of a given kind in the Hamiltonian. Already in the following work of Sheka in 1960 [14], done under the direction of Rashba, in the analysis of points of zero slope in crystals with zinc-blende structure, expressions were obtained by which, by the nature of the representation of the wave vector group, the wave function is transformed at the extremum, and the representation by which the operator is transformed gave the exact number of possible terms with such an operator in the Hamiltonian, taking into account the symmetry with respect to the operation of time inversion. What was lacking was a theory of the construction of the invariants themselves, which included, first of all, the construction of the basis matrices A_i of the irreducible representations by the known matrices of the irreducible representations of the group G_{k_o} . Such a theory was constructed by Pikus in 1961 and demonstrated on the example of the spectrum change in a deformed crystal with wurtzite structure [15,16], which can be characterized as a completion of the development of the invariant method for writing a general Hamiltonian from the symmetry properties of the crystal in a compact form with a strict definition of the number of possible invariants.

After the discovery of the dispersion law with a loop of extrema in crystals with wurtzite structure, Rashba together with his students Sheka and Boiko studied a lot the effects to which this law of dispersion leads (see Ref. [13]). As one of the brightest manifestations of this unusual law of dispersion a new kind of resonance was predicted by Rashba in 1960 [17,18], namely electro-dipole spin resonance (EDSR), in which transitions with spin change occur due to the electric component of the electromagnetic wave. The spin change without magnetic field was such an unusual result at that time that the experimenters who first observed this effect hesitated to publish it for a long time [19]. The existence of the EDSR was later confirmed experimentally for crystals with various kinds of symmetry. Rashba's work on EDSR was officially recognized as a discovery. To date, this resonance has been observed not only in bulk crystals of different symmetries, but also in low-dimensional structures, namely on heterojunctions and inversion layers, on dislocations and on impurity centers, which is described in detail in the review by Rashba and Sheka in 1991 [20]. The work of Rashba and his students on spin-orbit interaction had a great influence on the study of spin effects in both bulk and low-dimensional structures and became the basis of modern spintronics, which is described in detail in the review [13]. Fifty years after the paper [10] was published, in 2015, it was translated into English (because its Russian-language version was unavailable to the English-speaking scientific community) and named a “hidden jewel” in the review devoted to the Rashba effect [13].

II. METHOD OF INVARIANTS IN MODERN SOLID-STATE PHYSICS

Over the past half century, group theory has become an integral and in some sense routine part of solid-state theory (see for example Refs. [21,22]), and the method of invariants takes its honorable place here [23–25]. The method is effectively used for a very different class of problems, such as the motion of carriers in external electric and magnetic fields, changes in the energy spectrum under deformation, and many others, not only in bulk crystals and in low-dimensional structures [23,25], but in recent decades also for 2D crystals. For example, for graphene the invariants constituting the Hamiltonian were obtained for the first time in Winkler and Zúlicke's work in 2010 [26]. In this work, the method of invariants was employed not only to reproduce the linear spectrum of graphene at the K and K' points of the Brillouin zone—previously obtained only through tight-binding calculations—but also to derive higher-order terms in the wave vector $\mathbf{k}$ and additional Hamiltonian contributions induced by external electric

and magnetic fields, strain, and spin-orbit interaction. An anisotropic Fermi velocity renormalization by strain was predicted and later it was observed experimentally [27]. This work became the basis for the symmetry analysis of the band structure of not only graphene but other 2D crystals, such as silicene [28,29] and phosphorene [29], monolayer $X\text{Se}$ ($X = \text{In}, \text{Ga}$) [30] and MoS_2 [31], and others. For example, in paper [32] using the method of invariants the hyperfine interaction in transition metal dichalcogenide monolayers was described. This interaction was observed later for example in experiment [33].

In very recent years, symmetry-based methods and, in particular, the method of invariants [34–39] have been actively applied to the investigation of both three-dimensional and 2D crystals with complex magnetic and electric order. For example, in Ref. [34], symmetry analysis and the structure of invariants were used to predict a magnetic mechanism of SO coupling (the idea of intrinsic magnetic-field-induced spin splitting was originally proposed by Pekar and Rashba in 1964 [40]), demonstrated for the antiferromagnet MnF_2 . The resulting antiferromagnetic spin splitting is not related to the conventional electric SO coupling-induced spin splitting (Rashba-Dresselhaus) in nonmagnetic crystals and persists even in systems where electric SO spin splitting is absent. To date, experimental confirmation of such magnetic spin splitting has already been reported [41,42]. In Ref. [38], the symmetry approach and the method of invariants were applied to crystals with complex electric and magnetic order. Five categories of polarized matter were identified, and it was shown that each class can be characterized by a specific electronic band structure. For example, Rashba spin splitting in electropolar bulk materials such as wurtzite was explained in terms of electric polarization in such materials. In this work, a general formalism was developed, providing a physical interpretation and quantification of complex magnetic and electric order in crystals. Recently, this formalism has also been extended to chiral crystals [39].

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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