I. INTRODUCTION

The classical SO coupling enters into Schrodinger Hamiltonian describing electron (positron) motion in external potential from a non-relativistic approximation to the Dirac equation\(^1\). The famous Pauli term \(\frac{\hbar}{2m_e c}\sigma \cdot [V(r) \times \vec{p}]\) describes the renormalization of external potential acting on electron due to the presence of positron band. In order to describe kinetics of carriers in semiconductors in terms of elementary excitations - electrons/holes the single particle Schrodinger-like equations are to be extracted from multiband \(\vec{k} \cdot \vec{p}\) Hamiltonians. Usually this derivation follows the textbook pattern used in relativistic Dirac theory\(^1\). In what follows we are not going to discuss “pros and cons” of such approach but want to point out very important inconsistency of proposed derivation emerging at the start. This derivation relies on the validity of the assumption that some components of Dirac four-component wave function are responsible of and can be used for the description of electron/positron movement. Here we come up against the problem: even in the free of external forces space the movement of electron/positron by the definition is determined by all four components of wave function which are all indispensable for the description. The most striking example of such situation is the problem of velocity operator, known as Zitterbewegung\(^2\). The admixture of “non-proper” components results in “nonphysical” values of free electron velocity. One possible way to circumvent this problem is by making Foldy-Wouthuysen (FW) transformation, which allows to break the Dirac equation into separate equations for positive and negative energies\(^3\). But this approach suffers from drawback that FW transformation is not unique\(^4\). The same kind of difficulties are encountered while trying to obtain bound states in the field of supercharged nuclei in Dirac theory\(^1\).

It is commonly accepted that Dirac equation is not a single-particle equation and must be considered within quantum field theoretical approach. “The problem of charges in a fixed potential is usually treated by the method of second quantization of the electron field, using the ideas of the theory of holes.”\(^5\) The Dirac theory without second quantization is known to lead to interpretational problems and it is claimed that “single particle” paradoxes such as e.g. Klein effect are resolved if quantum field line approach is used\(^6\). Thus it seems logical to try to analyze the problem of single-particle equations in the field formulation. The more so, as only within such consideration the quantum number “charge” can be unambiguously ascribed to the given state described by multi-component wave function. Such approach allows to avoid along way possible arising of spurious superposition of negative and positive energy states as according to the famous statement “No one has ever succeeded in producing a state which is a superposition of states with different charges”\(^7\).

It was long established\(^8,9\) that “quasi-relativistic” problems infest any multiband semiconductor \(\vec{k} \cdot \vec{p}\) Hamiltonians. The reason lies in the fact that bulk band structure of semiconductors is frequently described within the framework of \(\vec{k} \cdot \vec{p}\) theory by matrix Hamiltonians which take into account at least two bands. Small wonder that if one proceeds along classical lines allowing for interference of positive and negative energy states such artefacts as effect of Zitterbewegung or Klein paradox emerge\(^9\). According to seminal paper by L. Keldysh\(^10\) the problem of supercharged nuclei transforms in semiconductors into the problem of deep levels of impurity centers.

In order to use electron/hole language in envelope function approximation we are to ascribe as in Dirac theory the quantum number “charge” to the single-particle eigenfunctions of appropriate multiband \(\vec{k} \cdot \vec{p}\) Hamiltonian. Thus it seems natural to carry out the quest for these equations on the field of second quantization. It must be noted that description of semiconductor properties within quantum field theoretical approach rare if ever appears in the literature\(^11\). The “inconvenience” of such line of approach for construction of single-particle
equations lies in the fact that such procedure can be carried out only in momentum representation. Thus instead of solving differential equations in coordinate space we are to solve integral equations. It must be mentioned that while this is to some extent new concept for solving multi-component envelope function problem, it was claimed that transition to momentum space allows to avoid ”spurious” solutions occurring in standard integration schemes\cite{12}. The second obstacle is that second quantization method is considered as an example of effective corrections do not in general coincide with commonly used one.

In what follows we start first of all with derivation of single-particle equations within proposed approach in “semiconductor” Dirac theory considering Dirac Hamiltonian as an example of the simplest two band $k \cdot p$ Hamiltonian. The obtained renormalized potential for Dirac-like semiconductors is compared with the classical (experimentally verified) expression for SO interaction, thus testing the validity of second quantization method for the solution of considered problem. Then we apply it to 2D Kane semiconductors with “positive” and “negative” energy gap.

It must be underlined that the term “SO” denoting sought correction to external potential in single-particle equations is used in the title and throughout the text in a broad sense. As it will be clear from the results presented below, physical origin and functional form of obtained corrections do not in general coincide with commonly used one.

\section{II. SO TERM IN 2D DIRAC-LIKE SEMICONDUCTOR}

Leaving aside pure relativistic problems Dirac Hamiltonian is considered as an example of effective $k \cdot p$ Hamiltonian, describing two-band semiconductor with symmetrical conduction and valence bands. The Dirac Hamiltonian has the following form

$$H_D = \begin{pmatrix}
\frac{E_x}{2} & \gamma k_+ & \gamma k_- \\
0 & \frac{E_z}{2} & -\gamma k_z \\
\gamma k_+ & -\gamma k_- & \frac{E_y}{2}
\end{pmatrix}, \quad (1)$$

where $k_\pm = k_x \pm ik_y$, $\gamma$ - characteristic velocity, $E_g$ - energy gap. In relativistic Dirac theory $E_g = 2mc^2$ and $\gamma = c$. Here and in the following the atomic units ($\hbar = 1$) are used.

To simplify the following analysis, we consider 2D version of Hamiltonian (1). Choosing $k_z = 0$ two groups of states ($\varepsilon 1/2, h - 1/2$) and ($\varepsilon -1/2, h 1/2$) do not mix. The Hamiltonian for the former group of these states reads

$$\hat{H}_D = \left(\begin{array}{cc}
\frac{E_x}{2} & \gamma k_+ \\
0 & \frac{E_y}{2}
\end{array}\right). \quad (2)$$

The Hamiltonian matrix for the second group of states is obtained by replacing $k_y$ by $-k_y$. Therefore, we consider only first group of states described by Hamiltonian (2). The energy eigenvalues of (2) are

$$\varepsilon(k)_{1,2} = \pm \sqrt{\frac{E_x^2}{4} + \gamma^2 k^2} \equiv \pm \varepsilon(k). \quad (3)$$

In the special case $E_g = 0$ Hamiltonian (2) is used for the description of electrons in $K$ valley in graphene

$$\hat{H}_K = \gamma \begin{pmatrix} 0 & k_- \\
\gamma k_+ & 0 \end{pmatrix}. \quad (4)$$

But in this case we do not have two groups of spin states. Instead we are dealing with pseudospin, which is a formal way of taking into account the two carbon atoms per unit cell. The Hamiltonian for $K'$ valley is obtained from (4) by making the transformation $\hat{H}_{K'} = - \hat{H}_K$.

In the second quantization picture the Hamiltonian (2) for intrinsic semiconductor is

$$\hat{H}_D = \int \varepsilon(k) \hat{a}^+(k) \hat{a}(k) d\mathbf{k} + \int \varepsilon(k) \hat{b}^+(k) \hat{b}(k) d\mathbf{k} . \quad (5)$$

Here $\hat{a}^+(k)$, $\hat{a}(k)$ are creation/annihilation operators for electrons and $\hat{b}^+(k)$, $\hat{b}(k)$ are corresponding operators for holes. Inserting the potential $V(r)$ into empty Hamiltonian diagonal, in accord with the commonly accepted prescription, we obtain the following additional terms in the Hamiltonian

$$\hat{H}_i = \int \int \varphi^*_e(k) \varphi_e(q) V(k-q) \hat{a}^+(k) \hat{a}(q) dkdq - \int \int \varphi^*_h(k) \varphi_h(q) V(k-q) \hat{b}^+(k) \hat{b}(q) dkdq + \int \int \varphi^*_e(k) \varphi_h(q) V(k-q) \hat{a}^+(k) \hat{b}(q) dkdq - \int \int \varphi^*_h(k) \varphi_e(q) V(k-q) \hat{a}(k) \hat{b}(q) dkdq. \quad (6)$$

where $\varphi_e(k)$, $\varphi_h(k)$ are eigen functions of (2) and

$$V(k) = \int V(r)e^{-ikr} dr. \quad (7)$$

The terms containing $\hat{a}^+(k) \hat{a}(q)$ and $\hat{b}^+(q) \hat{b}(k)$ describe the processes of scattering electrons/holes by the potential modified by the presence of filled valence band. The terms containing $\hat{a}^+(k) \hat{b}(q)$ and $\hat{a}(q) \hat{b}(k)$ describe the perturbation of vacuum (ground) state which is the necessary attribute of second quantized consideration.

The explicit expression for modified electron scattering
potential is
\[ V_e = \int \int N(k)N(q) \left( 1 + \frac{4\gamma k - q_+}{(E_g + 2\varepsilon(k))(E_g + 2\varepsilon(q))} \right) \times V(k - q) \hat{a}^+(k)\hat{a}(q)d\kappa dq, \]
where \( N(k) = \sqrt{\frac{E_g + 2\varepsilon(k)}{4\varepsilon(k)}} \). The expression for holes (positrons) is of the same functional form but has opposite sign.

It can be easily shown, that expansion of (8) up to the second order in \( \gamma k/E_g \ll 1 \) allows to present this expression as a sum of two parts

\[ V_e = \int \int V(k - q)\hat{a}^+(k)\hat{a}(q)d\kappa dq - \frac{\gamma^2}{2E_g^2} \int \int \left( 2i(k_x q_y - k_y q_x) - (k - q)^2 \right) \times V(k - q)\hat{a}^+(k)\hat{a}(q)d\kappa dq. \]

The inequality \( \gamma k/E_g \ll 1 \) means that characteristic “Compton” wavelength \( \lambda_C = \gamma/E_g \) is small as compared with the characteristic length of spatial variation of electron/hole envelope function \( \lambda = 1/k \). The condition \( \lambda_C \ll \lambda \) is always implied while considering semiconductor problems within effective mass approximation. In coordinate representation expression (9) has the following form

\[ V_e(r) = V(r) + \frac{\gamma^2}{E_g} \left[ \nabla V(r) \times \hat{p} \right] + \frac{\gamma^2}{2E_g^2} \mathbf{q}^2 V(r). \]

It is seen that renormalized electron scattering potential contains well known SO interaction term as well as Darwin term. It must be stressed, that the description of electrons and holes dynamics separately using such renormalized potential is possible if we neglect the pair production terms induced by external potential.

In the special case \( E_g = 0 \) (graphene) modified external potential has rather simple form

\[ \hat{H}_i = \frac{1}{2} \int \int \left( 1 + \frac{k - q}{k - q} \right) V(k - q)\hat{a}^+(k)\hat{a}(q)d\kappa dq - \frac{1}{2} \int \int \left( 1 + \frac{k + q}{k - q} \right) V(k - q)\hat{b}^+(q)\hat{b}(q)d\kappa dq + \frac{1}{2} \int \int \left( \frac{k + q}{k} - \frac{q - k}{q} \right) V(k - q)\hat{a}^+(k)\hat{b}(q)d\kappa dq - \frac{1}{2} \int \int \left( \frac{q - k}{k} - \frac{k - q}{q} \right) V(k - q)\hat{a}(q)\hat{b}(k)d\kappa dq. \]

The latter expression doesn’t depend on any band parameters of semiconductor, but only on the problem’s symmetry, thus demonstrating topological behavior.

In accord with the well-known result of Ref. 14, it is seen from (11) that back-scattering process \( k = -q \) is suppressed, as modified potential \( \left( 1 + \frac{k - q}{k - q} \right) V(k - q) \bigg|_{k = -q} = 0 \) for any potential, while pair production process is activated. This type of scattering process is similar to Andreev reflection15, in which initial electron passes the potential without scattering and simultaneously electron-hole pair is born.

Modified electron scattering potential (8) clearly has a non-local character in coordinate representation. To investigate further its properties let us write it down for the linear potential of the form \( V(r) = F \cdot x \)

\[ V_e = F \int \int \delta_{k_x q_y}(k, q)\hat{a}^+(k)\hat{a}(q)d\kappa dq - \frac{\gamma^2}{E_g} \int \int \frac{\gamma^2 k_y}{\varepsilon(k)(E_g + 2\varepsilon(k))} \hat{a}^+(k)\hat{a}(k)d\kappa , \]

where the linear potential in momentum representation is

\[ V(k - q) = F \cdot \frac{i}{2} \{ \delta_{k_y q_y}(k - q) - \delta_{q_y q_y}(q - k) \} = F \cdot \delta_{k_y q_y}(k, q). \]

The action of modifying term from (12) on a wave function of the form \( \Psi(x, y) = e^{\text{exp}(i q y)} \varphi(x) \) in coordinate representation is as follows

\[ \tilde{V}_{SO} \varphi(x) = \int K(x - x', q_y) \varphi(x')dx', \]

where

\[ K(\Delta x, q_y) = -F \int \frac{\gamma^2 q_y}{E_g} e^{ik_x \Delta x} dk_x. \]

In the limit \( ck/E_g \ll 1 \) the asymptotical behavior of the kernel \( K(\Delta x, q_y) \) is

\[ K(\Delta x, q_y) \sim \frac{\gamma q_y}{E_g} \left( 2e^{-\frac{q_y}{E_g} |\Delta x|} - e^{-\frac{q_y}{E_g} |\Delta x|} \right), \]

thus the smearing is determined by “Compton” wave length \( \gamma/E_g \). In the opposite limit \( E_g \to 0 \)

\[ K(\Delta x, q_y) \sim e^{-|q_y| |\Delta x|}, \]

i.e. the smearing is determined by de Broglie wave length \( 1/q_y \).

III. SO TERM IN 2D KANE SEMICONDUCTOR

The proposed approach is applied for the analysis of narrow gap semiconductors, described by Kane Hamiltonian16. In order to make mathematics less complicated and more descriptive the simplified version of Kane Hamiltonian is used, accounting only for \( \Gamma_6 \) and \( \Gamma_8 \) bands, while neglecting remote bands contribution. In 2D version of this Hamiltonian for \( k_z = 0 \) two groups of states \( (e 1/2, lh 1/2, hh - 3/2) \) and \( (e 1/2, lh - 1/2, hh 3/2) \) do not mix. The Hamiltonian matrix for the first group of these states in the case of
"positive" energy gap is
\[ \hat{H}_K = \begin{pmatrix} \frac{E_g}{2} & \frac{P}{\sqrt{2}} k_- & \frac{P}{\sqrt{2}} k_+ \\ \frac{P}{\sqrt{2}} k_+ & -\frac{E_g}{2} & 0 \\ 0 & 0 & -\frac{E_g}{2} \end{pmatrix}, \] (18)
where \( P \) - Kane’s momentum matrix element. The Hamiltonian matrix for the second group of states is obtained by replacing \( k_y \) by \(-k_y\). The energy eigenvalues of (18) are
\[ \varepsilon_{e, lh}(k) = \pm \frac{1}{2} \sqrt{E_g^2 + \frac{8}{3} P^2 k^2}, \] (19)
\[ \varepsilon_{hh}(k) = -\frac{E_g}{2}. \] (20)

It seen that the latter expression is similar to the one obtained for Dirac semiconductor. The coordinate representation equivalent of (21) is
\[ V_e(r) = V(r) + \frac{P^2}{3E_g^2} [\nabla V(r) \times \hat{p}]_z - \frac{P^2}{3E_g^2} \nabla^2 V(r) \] (22)

The obtained expression contains Rashba SO term\(^{17}\), as well as the term analogous to Darwin term. This result coincides with the one obtained in Ref. 18. Note one distinction of this expression from Dirac semiconductor. The prefactors ratio of SO and Darwin terms in the Dirac case is 2 : 1, while in the Kane case it is 1 : 1.

The situation with holes is more complicated. It has been already shown using purely group-theoretical methods that spin splitting for holes systems is very different from the spin splitting of electron states\(^{19}\). However we are not able to directly compare our results due to different problem’s geometry chosen.

The crucial difference from Dirac semiconductor case within our approach comes from the fact that we have two types of hole states. This means that interaction part of Hamiltonian contains diagonal terms \((\hat{a}^+(k)\hat{b}(q), \hat{b}^+_{lh}(q)\hat{b}_{lh}, \hat{b}^+_{hh}(q)\hat{b}_{hh})\), pair production terms \((\hat{a}^+(k)\hat{b}_{hh}(q), \hat{a}^+(k)\hat{b}^+_{hh}(q), \hat{a}(k)\hat{b}_{lh}(q), \hat{a}(k)\hat{b}_{hh}(q))\) as well as terms of the form \(\hat{b}^+_{lh}(q)\hat{b}_{hh}(k)\) and \(\hat{b}^+_{hh}(q)\hat{b}_{lh}(k)\). The latter terms describe the process of scattering between LH and HH states. Assuming the vacuum state to be stable, i.e. neglecting the electron-hole pair production terms, we obtain the following expression for the interaction part of effective Hamiltonian describing LH and HH behavior up to the second order in \(Pk/E_g\)
\[ H_i = -\int \int \left[ \frac{2P^2}{3E_g^2} k q + \frac{1}{k q} \left( 1 - \frac{P^2}{3E_g^2}(k^2 + q^2) \right) \left( k \cdot q - \frac{i}{2}(k_x q_y - k_y q_x) \right) \right] V(k - q) \hat{b}^+_{lh}(q)\hat{b}_{lh} dkdq \]
\[ -\int \int \frac{1}{k q} \left( k \cdot q + \frac{i}{2}(k_x q_y - k_y q_x) \right) V(k - q) \hat{b}^+_{lh}(q)\hat{b}_{hh}(k) dkdq \]
\[ -\int \int \frac{i\sqrt{3}}{2k q} \left( 1 - \frac{P^2k^2}{3E_g^2} \right) (k_x q_y - k_y q_x) V(k - q) \hat{b}^+_{lh}(q)\hat{b}_{lh}(k) dkdq \]
\[ -\int \int \frac{i\sqrt{3}}{2k q} \left( 1 - \frac{P^2q^2}{3E_g^2} \right) (k_x q_y - k_y q_x) V(k - q) \hat{b}^+_{lh}(q)\hat{b}_{hh}(k) dkdq. \] (23)

It is seen that terms describing scattering between LH and HH states are of the same order as diagonal ones.
As LH and HH states are of the same charge nothing forbids the interference between them which must be taken into account. Thus for hole system the single-particle Hamiltonian does not exist and renormalized potential is described by $2 \times 2$ matrix (see 23). The importance of taking into account the mixing of these two types of holes has been underlined in Ref. 10 while discussing the properties of deep levels in semiconductors.

Even the diagonal expression for modified LH $\rightarrow$ LH scattering potential qualitatively differs from the one obtained for electrons. It can’t be easily split into usual Rashba SO and Darwin-like terms. To further investigate properties of deep levels in semiconductors.

The latter expression contains usual SO term $\frac{P^2 k_y}{3E_g}$ as well as "topological" term $\frac{k_y}{2k}\delta_{q_x}$, which is similar to the one discovered in Dirac semiconductor case for $E_g = 0$.

The diagonal expression for modified HH $\rightarrow$ HH scattering potential doesn’t depend on band parameters of semiconductor and thus doesn’t have usual expansion parameter $Pk/E_g$. In the case of linear potential it is

\[
V_{hh} = F \int \int \delta'_{k_z,q_x}(k, q)\hat{b}_{hh}^+(q)\hat{b}_{hh}(k)dkdq \\
- F \int \left[ -\frac{k_y}{2k^2} + \frac{P^2 k_y}{3E_g} \right] \hat{b}_{hh}^+(k)\hat{b}_{hh}(k)dk . \tag{24}
\]

The latter expression contains the same "topological" $\frac{k_y}{2k}$ term as in LH case, but doesn’t have usual SO term.

At this point we can conclude that the origin of "topological" terms is the presence of degeneracy between LH and HH states at $\Gamma$ point. This statement was also confirmed while considering Dirac-like semiconductor in the case $E_g = 0$, where the same type of terms were found.

The Kane Hamiltonian for "negative" gap situation is obtained from (18) by simple change of $E_g$ sign. Thus it is easy to show that in doing so the eigenfunctions for LH and electron states are to be formally permuted with $k = -k$, while functional form of HH eigenfunction remains the same. Although the functions index interchange is a trivial matter, the physical consequences are far-reaching. As regards interaction of LH with external potential, it mimics the expression for electron SO in "positive" gap problem if electron-LH pair production is neglected

\[
V_{lh} = - \int V(k - q)\hat{b}_{lh}^+(q)\hat{b}_{lh}(k)dkdq \\
+ \frac{P^2}{3E_g} \int \left( i(k_xq_y - k_yq_x) + (k - q)^2 \right) \times V(k - q)\hat{b}_{lh}^+(q)\hat{b}_{lh}(k)dkdq . \tag{26}
\]

As in the case of electron interaction with external potential in Kane semiconductor with "positive" gap the obtained expression is of the "usual" Rashba form. The renormalized potential acting on electron and HH states is

\[
H_i = \int \left[ \frac{2P^2}{3E_g} kq + \frac{1}{k} \left( 1 - \frac{P^2}{3E_g} (k^2 + q^2) \right) \left( k \cdot q - \frac{i}{2} (k_xq_y - k_yq_x) \right) \right] V(k - q)\hat{a}^+(k)\hat{a}(q)dkdq \\
- \int \frac{1}{kq} (k \cdot q + \frac{i}{2} (k_xq_y - k_yq_x)) V(k - q)\hat{b}_{hh}^+(q)\hat{b}_{hh}(k)dkdq \\
- \int \frac{i\sqrt{3}}{2kq} \left( 1 - \frac{P^2 k^2}{3E_g} \right) (k_xq_y - k_yq_x) V(k - q)\hat{a}^+(k)\hat{b}_{hh}^+(q)dkdq \\
- \int \frac{i\sqrt{3}}{2kq} \left( 1 - \frac{P^2 q^2}{3E_g} \right) (k_xq_y - k_yq_x) V(k - q)\hat{a}(k)\hat{b}_{hh}(q)dkdq . \tag{27}
\]

It is seen that in this case the SO interaction for electrons can’t be described by Rashba-like expression. Instead due to degeneracy of electron and HH bands scattering potential has "topological" terms contribution. Moreover pair production process can’t be neglected, which makes this case similar to Dirac semiconductor case when $E_g = 0$ (graphene). Another difference from "positive" gap case is that in this case scattering process between LH and HH states can be neglected since LH and HH band are separated by energy gap.
IV. SUMMARY

The derivation of Schrodinger-like single-particle equations describing electron/hole dynamics in external potential in intrinsic 2D Dirac and Kane semiconductors was carried out within second quantization method. Such approach allows automatically to take into account the effect of filled valence bands and to avoid in the cause of derivation unphysical superposition of positive and negative energy states. It is shown that obtained modified potential entering the sought equations may differ essentially from its classical “SO” counterpart as in its functional form, so in its dependence on band parameters. The degenerate bands modification of potential is very strong due to the presence of “topological” terms which do not depend on band parameters. Such strong modification of potential leads for instance to the absence of back-scattering in 2D Dirac problem, to the mixing of LH and HH states dependent only on the strength of potential in “positive” gap Kane problem and to the strong perturbation of valence vacuum in the proximity of potential in “negative” gap case. Moreover in coordinate representation the modified potential leads for instance to the absence of LH and HH states dependent only on the strength of back-scattering in 2D Dirac problem, to the mixing of potential in Schrodinger-like equation, if it exists, is in general represented by non-local operator in all considered problems. This raises the interpretational issue. The generally accepted physical interpretation of SO origin is that it is a result of interaction of intrinsic electron/hole magnetic moment (spin) with magnetic field induced by orbital motion of the particle in external potential. Such “classical” interaction if of course presumed to be local. In our case the effective single-particle potential is renormalized in such a way as to exclude scattering of the electrons into occupied valence states. Thus it is reasonable to consider it as some kind of pseudo potential which actually does not differ in essence from the ones used in solid state physics. The presented approach show that SO terms understood as the renormalization of potential in single-particle equations arises whenever we are dealing with two or more interacting energy bands. It is interesting that the similar statement was made in Ref. 9 while discussing the nature of Zitterbewegung. From this point of view the external potential renormalization is not necessary related to spin. E.g. consider graphene case where intrinsic SO interaction is extremely small, however the effect of external potential renormalization still takes place. As it was pointed above in order to remain within single-particle description (if possible) the terms leading to pair producing process must be disregarded. According to Schwinger the pair production process is activated when the work of external potential along Compton length exceeds . For instance in a typical narrow gap semiconductor with and external electric field has to exceed 10^7 V/m.

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