The quantum mechanical probability density and probability current density operators in the Pauli theory

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We present systematic construction of probability and probability current densities operators for one-band single particle Pauli equations starting from the operators in Dirac electron model within Second Quantized Approach. These operators are of importance as in probability interpretation of experimental data, so in establishing of boundary conditions. It is shown that derived operators differ significantly from their conventional Schrodinger-type counterparts. The generalization of continuity equation for probability density under external perturbations and physical meaning of additional source terms is discussed. The presented approach can be useful in analysis of carriers dynamics described within generic multicomponent $k \cdot p$ Hamiltonians in Envelope Function Approximation (EFA).

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I. INTRODUCTION

The quantum mechanical concept of probability and probability current density is of utter importance for interpretation of experimental results connecting the wave-like description of the quasiparticle with macroscopic observables [1]. In non-relativistic quantum mechanics the functional form of these quantaties, as their physical interpretation, accompanying the solution of corresponding Schrodinger equation, are well established. Nevertheless, in the general case, the quantum behavior of electron under external perturbation must be described by relativistic Dirac equation [2]. The revival of interest in Dirac equation is triggered also by recent advances in spintronics and new developments in condense matter systems, especially with advent of graphene. It was shown that there exist an analogy between the Dirac description of electron kinetics in vacuum and the coupled-band formalism for electrons in narrow-gap semiconductors and carbon nanotubes [3]. At the same time, the relativistic Dirac equation poses major open problems which are due to the presence of negative energy spectrum interpreted as antimatter (positrons). It is of common consensus that the so-called single-particle solutions of Dirac Hamiltonian describe not so much particle states as the states with the charge $\pm e$ which are in general multiparticle states [4]. Relativistic corrections to electron dynamics are taken into account in quantum chemistry calculations, especially for systems containing heavy elements [5]. Nevertheless, the relativistic approach based on Dirac-Kohn-Sham equations and Dirac-Hartree Fock models [6, 7] is too complex in general to handle either analytically or numerically [8]. Thus semirelativistic one-band description of electron behavior described by so called two-component Pauli equation, which is much simpler to solve, is very popular. The problem of approximate reduction of four component Dirac problem to two component Pauli problem is solved usually by the projection method proposed by Foldy and Wouthuysen (FW) [9] and its modifications, or by so called elimination method of Pauli [10]. As a result the electron and positron (hole) degrees of freedom are formally disentangled in Dirac Hamiltonian and their dynamics is described separately by two spinor Pauli-like equations. While FW approach is without doubt valid for “free” Dirac problem, it comes into conflict with Quantum Field description in general, when external perturbation is switched on. FW approximation ignores the possibility (inevitable in this case) of real/virtual pair creation processes. Simultaneously with formulation of Pauli-like equations, there arises the question of relativistic corrections to Schrodinger probability and current. Usually, the sought for expressions are obtained starting from second-order in $1/c$ Hamiltonian, obtained through FW transformation [1, 11].

We intend to show, that straight and physically clear way to derive the form of probability and probability current densities operators supplementing two-component Pauli-like equations is to view this problem upon within the second quantization method (SQM) consized as an alternative to FW-type approach. This is not at all new approach to the derivation of Pauli equation [12–14]. Nevertheless, this approach has not been applied for derivation of the form of single particle probability and probability current density operators in Pauli theory starting from their counterparts in Dirac theory. At the same time, these quantities are crucial for formulation of boundary conditions and probability interpretation of experimental data. In what follows we adopt the simplest “no-pair” approximation, neglecting possible pair production while projecting Dirac operators onto single particle channel.

The paper is organized as follows. In Sec. III and Sec. III we derive the probability density and probability current operators respectively. In Sec. IV we discuss the peculiarities of obtained probability continuous equation.
II. PROBABILITY OPERATOR

The four component spinors of plane-wave eigenfunctions of free problem, described by Dirac Hamiltonian $H_D = c\alpha \mathbf{k} + \beta mc^2$ are chosen for positive energy branch ($\hbar = 1$) in momentum representation as

$$u_{k,1} = \sqrt{\frac{\varepsilon + 1}{2\varepsilon}} \begin{pmatrix} 1 \\ \frac{\lambda_C \varepsilon + i}{\varepsilon + 1} \end{pmatrix}, \quad u_{k,2} = \sqrt{\frac{\varepsilon + 1}{2\varepsilon}} \begin{pmatrix} 1 \\ 1 \frac{\lambda_C \varepsilon + i}{\varepsilon + 1} \end{pmatrix},$$

and for negative branch the eigen functions are

$$\tilde{u}_{k,1} = \sqrt{\frac{\varepsilon + 1}{2\varepsilon}} \begin{pmatrix} 1 \\ -\frac{\lambda_C \varepsilon + i}{\varepsilon + 1} \end{pmatrix}, \quad \tilde{u}_{k,2} = \sqrt{\frac{\varepsilon + 1}{2\varepsilon}} \begin{pmatrix} 1 \\ 0 \frac{\lambda_C \varepsilon + i}{\varepsilon + 1} \end{pmatrix},$$

where $\lambda_C = 1/mc$, $\varepsilon = \sqrt{1 + \lambda_C^2 k^2}$. We will need also “bare” plane-wave representation spanned by the following set of four-component spinors

$$u_{k,1}^0 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad u_{k,2}^0 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \tilde{u}_{k,1}^0 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \tilde{u}_{k,2}^0 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix},$$

Where $u_{k,1}^0, u_{k,2}^0$ represent “bare” electron states and $\tilde{u}_{k,1}^0, \tilde{u}_{k,2}^0$ are “bare” hole states. This representation is needed as only within this representation in position space the momentum operator is obtained by replacing $k \rightarrow -i\nabla$ and position operators are $\epsilon$-numbers. The same substitution is used for the solution of multiband $k \cdot p$ Hamiltonians within EFA. Thus the semiconductor problems become analogous to the ones in the relativistic theory [12], allowing to extend the obtained below results in Dirac theory to the description of carriers in semiconductors [13].

The field operator can be decomposed into “dressed” creation/annihilation electron/hole operators, diagonalizing free $H_D$, or into “bare” creation/annihilation operators, diagonalizing free $H_D$, or into “bare” ($a_{k,i}^+, a_{k,i}^-, b_{k,i}^+, b_{k,i}^-$) ones.

$$\Psi(r) = \int \left( u_{k,1}^0 a_{k,1} + u_{k,2}^0 a_{k,2} + \tilde{u}_{k,1}^0 a_{k,1} + \tilde{u}_{k,2}^0 a_{k,2} \right) \times e^{i\mathbf{kr}} \, dk$$

$$= \int \left( u_{k,1} a_{k,1} + u_{k,2} a_{k,2} + \tilde{u}_{k,1} B_{k,1}^+ + \tilde{u}_{k,2} B_{k,2}^+ \right) \times e^{i\mathbf{kr}} \, dk$$

Using [5] it is straightforward to write down Bogoliubov transformation from “bare” to “dressed” operators

$$\begin{align*}
(a_{k,1}, a_{k,2}) &= N_k I \left( A_{k,1}, A_{k,2} \right) - M_k \lambda_C \sigma \cdot k \left( B_{k,1}^+, B_{k,2}^+ \right), \\
(b_{k,1}, b_{k,2}) &= N_k I \left( B_{k,1}^+, B_{k,2}^+ \right) + M_k \lambda_C \sigma \cdot k \left( A_{k,1}, A_{k,2} \right),
\end{align*}$$

The probability density operator $\hat{P}(\mathbf{R})$ by definition is

$$\hat{P}(\mathbf{R}) = \int \Psi(r)^\dagger \delta(\mathbf{R} - r) \Psi(r) dr.$$

Inserting Dirac field operator [5] into the latter expression we obtain

$$\hat{P}(\mathbf{R}) = \frac{1}{(2\pi)^3} \sum_{s=1,2} \int \left( a_{k+q,s}^+ a_{k,s} + b_{k+q,s}^+ b_{k,s} \right)$$

$$\times e^{i\mathbf{qR}} dkdq = \frac{1}{(2\pi)^6} \int \hat{P}(\mathbf{q}) e^{i\mathbf{qR}} dq.$$
In gapless case ($\lambda_C \to \infty$ or $m \to 0$), which can be of interest while analyzing the behavior of carriers in quazi-relativistic "graphene" case, this expression simplifies to

$$
\hat{P}_e(q) = \frac{1}{2} \int dk \left[ \left( A_{k+q,1}^+ A_{k+q,2}^+ \right)^T \left( 1 + (n_k \cdot n_{k+q}) \right) + i \sigma \cdot [n_k \times n_{k+q}] \right] \left( A_{k,1} \right) \left( A_{k,2} \right),
$$

(13)

where $n_k = k/|k|$. It is seen from [13] that probability of electron scattering from the state $|k\rangle$ to the state $|-k\rangle$ ($q = -2k$) is zero. This is manifestation of the well-established fact that backscattering is absent in 3D Weyl or 2D graphene [19] case. It must be stressed that this result does not depend on the form of external perturbation. This is an inherent property of the defined probability operator and is a consequence of introducing vacuum (filled valence band in $k \cdot p$ theory) into the Dirac theory. Note, that this result is valid in our approach only if we impose the condition of vacuum stability. It must be stressed that in the gapless case the separation of modified potential in Pauli equation into "bare" and SO parts is meaningless. As it is seen from [13], all three terms, including "bare" potential term, are of the same order and do not depend on the parameters of the problem, but only on the strength of external potential.

As we intend to apply proposed approach elsewhere for constructing density and current operators in semiconductors described within multi-component $k \cdot p$ Hamiltonians, it is of interest to consider low energy limit $\lambda_C k \ll 1$. In $k \cdot p$ theory such approximation is known as EFA, while in Dirac theory it is called $1/c$ approximation [2] or $v/c$ approximation [16]. As it will be seen this approximation not only simplifies the derived expressions but allows the elucidation of the physical meaning of various terms entering obtained expressions. Using the approximate expressions for $N_k$ and $M_k$ up to the second order in $\lambda_C k$

$$
N_k \approx 1 - \frac{1}{8} \lambda_C^2 k^2,
$$

(14)

$$
M_k \approx \frac{1}{2} \left( 1 - \frac{3}{8} \lambda_C^2 k^2 \right),
$$

(15)

$$
\varepsilon_k \approx 1 + \frac{1}{2} \lambda_C^2 k^2 - \frac{1}{8} (\lambda_C k^2)^2,
$$

(16)

the expression for $\hat{P}_e(q)$ simplifies to

$$
\hat{P}_e(q) = \sum_{s=1,2} \int dk \left[ \left( A_{k+q,s}^+ \right)^T \left( 1 - \frac{1}{8} \lambda_C^2 q^2 \right) A_{k,s} \right] \left( A_{k,1} \right) \left( A_{k,2} \right) + i \frac{\lambda_C^2}{4} \int dk \left( A_{k+q,1}^+ A_{k+q,2}^+ \right)^T \sigma \cdot [q \times k] \left( A_{k,1} \right) \left( A_{k,2} \right).
$$

(17)

It is widespread opinion that in Pauli equation, considered as non-relativistic approximation to Dirac equation, the probability density remains Schrödinger-like equal to $|\Psi(r)|^2$, where $\Psi(r)$ is an appropriate wave function. It is stated that for free spin one-half particle only probability current density undergoes modification and spin-dependent divergenceless term

$$
\frac{1}{2m} \left[ \nabla \times (\Psi^\dagger(r) \sigma \Psi(r)) \right]
$$

(18)

is added to classical Schrödinger expression [11, 20]

$$
\frac{1}{2m} \left( \Psi^\dagger(r) \nabla \Psi(r) - \Psi(r) \nabla \Psi^\dagger(r) \right).
$$

(19)

As seen from [17] the derived Pauli probability density operator also differs essentially from its canonical counterpart. In order to understand the meaning of obtained result let us consider the probability density $W(R)$, that is by the definition

$$
W_e(R) = \int \langle \varphi(k)|\hat{P}_e(R)|\varphi(r)\rangle dr = \frac{1}{(2\pi)^6} \int \langle \varphi(k+q)|\hat{P}_e(q)|\varphi(q)\rangle e^{-iqR} dk dq.
$$

(20)

Here the averaging is done over single particle functions of the type

$$
|\varphi(k)\rangle = |\varphi_1(k)A_{k,1}^+ + \varphi_2(k)A_{k,2}^+|0\rangle
$$

(21)

and it is assumed that

$$
\int \langle |\varphi_1(k)|^2 + |\varphi_2(k)|^2 \rangle dk = 1.
$$

(22)

Let us consider expansion of $W_e(R)$ up to the second order in $\lambda_C k$. The "classical" result is reproduced in the zeroth order in $\lambda_C k$.

$$
\delta W_{e,0}(R) \approx \int [\varphi_1^*(k+q)\varphi_1(k) + \varphi_2^*(k+q)\varphi_2(k)] e^{-iqR} dk dq = |\varphi_1(R)|^2 + |\varphi_2(R)|^2.
$$

(23)

The account of terms of the second order in $\lambda_C k$ leads to the following additional spin independent term $\delta W_{e,1}(R)$ and spin dependent term $\delta W_{e,2}(R)$

$$
\delta W_{e,1}(R) = -\frac{1}{8} \lambda_C^2 \Delta \Psi^\dagger(R) \Psi(R),
$$

(24)

$$
\delta W_{e,2}(R) = -\frac{i}{4} \lambda_C^2 (\nabla_{r_1} \times \nabla_{r_2}) \Phi^\dagger(r_1) \sigma \Phi(r_2)|_{r_1 = r_2 = R},
$$

(25)

Here $\Phi(R)$ is two component Pauli spinor

$$
\Phi(R) = \left( \begin{array}{c} \varphi_1(R) \\ \varphi_2(R) \end{array} \right).
$$

(26)

The similar terms for the charge and current densities
considered as the sources in the Maxwell equations were obtained in [3]. The derivation within Lagrangian approach, which is valid up to the second order in $\lambda_C k$, was based on a two component Pauli-like equation obtained by Foldy-Wouthuysen transformation.

We can use our density operator to incorporate external field into Pauli equation. The expectation value of interaction with the classical potential field $V(R)$ in electron sector can be written as

$$\int V(R)W_e(R)dR. \quad (27)$$

The spin independent terms $\delta W_{e,1}(R)$ and $\delta W_{e,2}(R)$ generate classical Schrodinger potential term

$$\int V(R)\Phi^\dagger(R)\Phi(R)dR \quad (28)$$

and Darwin term

$$\frac{1}{8}\lambda_C^2 \int \Phi^\dagger(R)\Delta V(R)\Phi(R)dR. \quad (29)$$

The spin dependent term generates spin-orbit interaction term

$$\frac{1}{4}\lambda_C^2 \int \Phi^\dagger(R)|\nabla V(R)\times \mathbf{p}|\Phi(R)dR. \quad (30)$$

Thus within proposed approach, it follows that the external potential modification is contained implicitly in the “proper” defined density probability expression, owning its complicated form to the account for the existence of vacuum (filled valence band). It must be stressed that we can arrive at the same result within projection operator approach (Foldy-Wouthuysen method) in the considered $\lambda_C$ approximation. Within our approach the general expression for spin-dependent contribution to probability density operator, responsible for Rashba-like interaction, predicts non linear dependence on wave vector $\mathbf{21, 22}$. More generally, for arbitrary potential its interaction with spin is non-local. Really, using $\mathbf{12}$ we obtain the following term in Pauli Hamiltonian

$$\Delta H_{SO} = i\lambda_C^2 \int \Phi^\dagger(k+q)V(q)\sigma \cdot [q \times k] \Phi(k)dkdq, \quad (31)$$

where $\Phi(k) = M_k \Phi(k)$. In configuration space $\Delta H_{SO}$ can be written as

$$\Delta H_{SO} = \lambda_C^2 \int \Phi^\dagger(R_1)\hat{H}_{SO}(R_1, R_2)\Phi(R_2)dR_1dR_2, \quad (32)$$

where non-local operator $\hat{H}_{SO}(R_1, R_2)$ is

$$\hat{H}_{SO}(R_1, R_2) = \int K(R_1 - R)\hat{H}_{SO}(R)K(R - R_2)dR. \quad (33)$$

where $\hat{H}_{SO}(R)$ is familiar SO operator

$$\hat{H}_{SO}(R) = \sigma [\nabla V(R) \times \mathbf{p}]$$

and

$$K(R) = \int M_k e^{-ikR}. \quad \text{Alternatively, the arrived result can be viewed upon as the “smearing” of the wave function. Within both interpretations the physical origin of the effect can be attributed to peculiarity of position operator in relativistic Dirac theory. As it has been shown in $\mathbf{23}$ in Dirac theory the position operator must be considered as a non-local integral operator in configuration space. We can arrived to the same conclusion within Foldy-Wouthuysen approach $\mathbf{24}$. It was shown that within our alternative approach it can be inferred that position operator components do not commute in general $\mathbf{17}$. Thus any function of coordinates becomes operator and consequently will be “smeared” as regards its classical counterpart due to emerging uncertainty relation. The spatial behavior of the “smearing” kernel $K(R)$ can be estimated following the line of arguments of $\mathbf{25}$}. The transformation kernel in 3D case can be written as

$$K(R) = \frac{1}{(2\pi)^3} \int \frac{e^{ikR}}{\sqrt{2\varepsilon_k (\varepsilon_k + 1)}}dk, \quad (34)$$

where $G(k) = \sqrt{\varepsilon_k}/\sqrt{2(\varepsilon_k + 1)}$. This function varies very slowly from $G(0) = 0.5$ to $G(\infty) = 1/\sqrt{2} \approx 0.707$. Thus, following $\mathbf{25}$ we approximate $G(k)$ by some effective constant $G_0$. Using the following expressions $\mathbf{26}$

$$\int_{-\infty}^{\infty} \frac{e^{itz}}{\sqrt{t^2 + a^2}}dz = 2K_0(az), \quad (35)$$

$$\int_0^\infty tJ_0(\beta t)K_0(\alpha \sqrt{t^2 + 1})dt = \frac{K_1(\sqrt{\alpha^2 + \beta^2})}{\sqrt{\alpha^2 + \beta^2}}, \quad (36)$$

where $K_1(z)$ is the modified Bessel (Mac Donald) function, we obtain

$$K(R) \approx \frac{G_0}{2(2\pi)^2\lambda_C^2} \frac{\lambda_C}{R} K_1 \left( \frac{R}{\lambda_C} \right). \quad (37)$$

Using asymptotic behavior of $K_1(z) \mathbf{27}$

$$K_1(z) \approx \sqrt{\frac{\pi}{2z}} e^{-z} \left( 1 + O \left( \frac{1}{z} \right) \right). \quad (38)$$

We see that the smearing wave function (potential) function have a finite width of the order of $\lambda_C$.

In 2D case the kernel describing non-local interaction with external potential within the same approximation
The truncation to electron channel leads to the following
and negative energies. So, the proposed approach must
existance of two different types of states with positive
and negative energies. So, the proposed approach must
be valid for the analysis of \( k \cdot p \) problems, which are by
the definition considered in the fixed rest frame of crystal.

Two main aspects of proposed form of probability den-
sity operator must be underlined. As it was shown, all
information about “relativism” (SO-like and Darwin-like
terms) is contained in defined probability density oper-
ator, while external potential is considered as classical.
Secondly, the obtained functional form of probability op-
erator implies that wave function, obtained as the solu-
tion of derived two-component Pauli equation, plays sub-
sidiary role. The probabilistic interpretation of outcome
of experiment is given by averaged value of found prob-
ability density operator over the corresponding single par-
ticle wave functions, which are the solutions of Pauli-like
equation. One more reson for implementation of second
quantization scheme will be justified below while consid-
ering the time dependence of density operator, which is
crucial for formulation of continuity equation.

III. CURRENT DENSITY OPERATOR

Following the outlined procedure the charge current
density operator in Dirac theory is by the definition in
bare representation is

\[
\hat{J}(q) = c \int \Psi^+(r) \alpha \delta(R - \hat{r}) \Psi(r) e^{-iqR} dr dR
\]

\[
= c \int \left[ \begin{array}{c} a_{k+q,1}^T \sigma (b_{k,1}^T) + (b_{k+q,1}^T) \sigma (a_{k,1}) \\ a_{k+q,2}^T \sigma (b_{k,2}^T) + (b_{k+q,2}^T) \sigma (a_{k,2}) \end{array} \right] dk.
\]

(39)

The truncation to electron channel leads to the following
expression

\[
\hat{J}_e(q) = c \int N_{k+q} M_{k+q} \lambda \left( A_{k+q,1}^T \sigma (\sigma \cdot k) A_{k,1} \right) dk
\]

\[+ c \int N_{k+q} M_{k+q} \lambda \left( A_{k+q,2}^T \sigma \cdot (k + q) A_{k+2}^T \sigma \cdot A_{k,1}^T \right) dk
\]

\[= \hat{J}_{1,e}(q) + \hat{J}_{2,e}(q) + \hat{J}_{e,Z}(q),
\]

(40)

where

\[
\hat{J}_{1,e}(q) = c \lambda c \sum_{s=1,2} \int dk \left[ N_{k+q} M_{k+q} \right.
\]

\[+ N_{k+q} M_{k+q,1} (k + q) A_{k+q,1}^T A_{k,2}^T \right) \sigma \cdot A_{k,1}.
\]

(41)

\[
\hat{J}_{2,e}(q) = ic \lambda c \int dk \left[ N_{k+q} + M_{k+q} \right.
\]

\[+ N_{k+q} M_{k+q} \left( A_{k+q,1}^T A_{k+q,2}^T \right) [k \times \sigma \cdot (A_{k,1}^T A_{k,2})].
\]

(42)

\[
\hat{J}_{e,Z}(q) = -ic \lambda c \int dk N_{k+q} M_{k+q} \left( A_{k+q,1}^T A_{k+q,2}^T \right) [q \times \sigma \cdot A_{k,1}]^T A_{k,2}.
\]

(43)

The first term \( \hat{J}_{1,e}(q) \) in the zero order approximation in
\( \lambda C k \) is

\[
\hat{J}_{1,e}(q) \approx \frac{1}{2m} \lambda c \sum_{s=1,2} \int dk [2k + q] A_{k+q,1}^T A_{k,2}.
\]

(44)

It is easy to recognize “classical” result in this term after
averaging over corresponding wave functions

\[
\int \langle \varphi(r) | \hat{J}_{1,e}(q) | \varphi(r) \rangle \, dr
\]

\[= -\frac{i}{2m} \left( \Psi^T(R) \nabla \Psi(R) - \Psi(R) \nabla \Psi^T(R) \right).
\]

(45)

The last divergenceless \( (q \cdot \hat{J}_{e,Z}(q) \equiv 0) \) term \( \hat{J}_{e,Z}(q) \)
represents so called spin magnetization current. The
necessity of its presence was established long ago by
G. Breit\[26\]. The addition of this current in considered
approximation to the classical Schrodinger expression has
been justified in \[8,20\]. The necessity for accounting of
this term in current is supported by the fact that the Zee-
man term arises due to it in Pauli Hamiltonian. Really,
by choosing

\[
A(R) = \frac{1}{2} [B \times R]
\]

for constant magnetic field \( B \), the corresponding term
in expression for expectation value of interaction with
external electromagnetic field is

\[
H_{Z,1} = \frac{e}{c} \sum_{s=1,2} \int A(R) \langle \hat{J}_{e,Z}(q) | e^{-iqR} dq dR
\]

\[= i \frac{e}{2c} \int [B \times \nabla \delta(q)] \langle \hat{J}_{e,Z}(q) | dq.
\]

(46)

After some manipulation using well-known equality

\[
[A \times B] [C \times D] = (AC)(BD) - (AD)(BC)
\]

and expression \[43\], the expectation value of interaction
with external electromagnetic field can be presented as
the Zeeman term

\[ H_{Z,1} = \frac{e}{2mc} \int \frac{B\sigma}{m\varepsilon_k} dk. \]  

(48)

Note that in relativistic mechanics \(\varepsilon_k = \sqrt{1 - v^2/c^2}\). This result means that in Zeeman term the rest mass in the expression for spin magnetic moment of Pauli electron must be replaced by expectation value of energy-dependent Lorentz mass in the corresponding quantum state. Compare this result with [29]. The \(\lambda_C^2\) expansion of this expression up to the second order produces the relativistic correction term to the Zeeman interaction \(g\mu B\)

\[ H_{Z,1} \approx -\frac{e}{4mc} \lambda_C^2 \int (k^2 B\sigma) dk. \]  

(49)

This addition to intrinsic magnetic moment due to the \(k^4/8m^2c^2\) term in expansion of relativistic kinetic energy was considered in [30]. This dependence of mass on velocity must be accounted for if spin-orbit interaction is taken into account, as its contribution to single particle Hamiltonian is of the same order in \(\lambda_C^2\).

Nevertheless this result cannot be considered as final. The point is that there is additional spin-dependent term \(\mathbf{J}_{S,Z}(q)\), depending also on \(B(r)\), but not explicitly on \(A(r)\). Thus it must be added to written above Zeeman term.

\[ H_{Z,2} = \frac{e}{2mc} \int \langle k \times \sigma | \hat{N}_{k+q} M_k - M_{k+q} \hat{N}_k \rangle \rangle \int (B|k\sigma) dk dq \]

\[ = \frac{3}{4} \lambda_C^2 \left( \frac{(B|k\sigma) - (B|\sigma)k^2}{\varepsilon_k^2(1 + \varepsilon_k)} \right) \]

\[ = -\frac{e}{2c} \langle \Delta \hat{S}_{FW} B \rangle, \]  

(50)

It is easy to recognize in the term \(\Delta \hat{S}_{FW}\) the one appearing in spin operator of Foldy-Wouthuysen theory. In accord with our no-pair approximation we retain only even part \(\hat{S}_{FW}^{\text{even}}\) of defined by them spin operator \(\hat{S}_{FW}\) which is in our notation

\[ \hat{S}_{FW}^{\text{even}} = \frac{1}{2} \sigma - \frac{1}{2} \lambda_C^2 \frac{k \times [\sigma \times k]}{\varepsilon_k(1 + \varepsilon_k)}. \]  

(51)

For massless situation describing charged “neutrinos” (graphene case) the Zeeman term is

\[ H_{Z,1} = \frac{1}{2} e \int \frac{\langle B \times \sigma \rangle}{|k|^2} dk, \]  

(52)

\[ H_{Z,2} = \frac{1}{2} e \int \frac{\langle B \times k \rangle |k \times \sigma|}{|k|^2} dk. \]  

(53)

IV. CONTINUITY EQUATION

In the first quantization scheme the probability density current in Dirac theory \(\hat{J}(k, t) = c \alpha \exp(-i\mathbf{k}\cdot\mathbf{r}(t))\) is connected with the probability density \(\hat{P}(k, t) = \exp(-i\mathbf{k}\cdot\mathbf{r}(t))\) via continuity equation

\[ \frac{\partial \hat{P}(k, t)}{\partial t} = i[\hat{H}, \hat{P}(k, t)] = -i \mathbf{k}\cdot\mathbf{r}(t). \]  

(54)

The time dependence of \(\hat{P}(k, t)\) in the Heisenberg representation is determined in SQM by the time dependence of creation/annihilation operators. In the free of external perturbations Dirac problem

\[ A_k(t) = e^{-imc^2\varepsilon_k t} A_k, \]  

(55)

\[ A_k^+(t) = e^{imc^2\varepsilon_k t} A_k^+. \]  

(56)

Thus, the time derivative of \(\hat{P}(k, t)\) is

\[ \frac{\partial \hat{P}_c(q, t)}{\partial t} = imc^2 \sum_{s=1, 2} \int (\varepsilon_{k+q} - \varepsilon_k)[N_{k+q} N_k + M_{k+q} M_k \lambda_C^2 ((k + q) \cdot k)] A_{k+q,s}(t) A_{k,s}(t) dk \]

\[ - \frac{1}{m} \sum_{s=1, 2} \int M_{k+q} M_k (\varepsilon_{k+q} - \varepsilon_k) \left( A_{k+q,1}(t) \sigma \cdot [q \times k] A_{k,1}(t) \right) A_{k+q,2}(t) \]

The “Zeeman” current \(\mathbf{J}_{Z,2}(q, t)\) being divergenceless does not contribute to the continuity equation. Nevertheless, it must be retained because it is responsible for Zeeman interaction.

As the Dirac probability current density \(\alpha \delta(R - \mathbf{r})\) is not affected by switching on of electromagnetic field, the famous term \(\mathbf{A}(r)\Psi^*(r)\Psi(r)\) can not appear in our non-relativistic expression for Pauli current. Nevertheless, this term is essential for the conserving of the gauge invariance. So, the question arises where do we lost it? The point is that we have not taken into account changing of equations of motion for annihilation/creation operators due to the Peierls substitution \(\mathbf{p} - \frac{e}{c} \mathbf{A}(r)\), when electromagnetic field is switched on. It can be shown in our approach, that the following term appears accordingly in single particle Pauli equation (in the first order in pa-
The first paramagnetic contribution to the current is set to zero assuming rigidity of macroscopic superconductor wave function and in another words proposing the stability of Bose vacuum of Couper pairs under external perturbation. The second diamagnetic term, dependent on vector potential, is considered to be different from zero and describes the penetration of external magnetic field into superconducting media. It must be noted once more, that obtained within proposed approach simple form \( \rho_{div} \) of material current is valid only in the zeroth approximation in \( \lambda C k \). In general, the expression for this current depends non-locally on the vector potential in position space. There is a different approach to the derivation of probability current density outlined in classic textbook of Landau and Lifshitz [34]. It is based on vector potential variation of phenomenologically written down approximate Pauli equation for electron. While their approach gives the same expression for \( J_e \), it does not reveal the essential physical difference in the origin of these two contributions.

If the external scalar potential perturbation \( V(r) \) is applied to the system, the equations of motion for creation/annihilation operators are governed in electron channel by the Hamiltonian

\[
\hat{H}_e = \hat{H}_{0,e} + \hat{H}_{int,eV},
\]

where \( \hat{H}_0 \) - the Hamiltonian of free Dirac problem and \( \hat{H}_{int,eV} \) is of the form

\[
\hat{H}_{int,eV} = \sum_{s=1,2} \int V(q) \left[ N_{k+q}N_k + M_{k+q}M_k((k+q)\cdot k) \right] A^+_k A_{k,s} \, dk \, dq
\]

\[
+ \int V(q) \, M_{k+q} M_k \left( \begin{array}{c} A^+_{k+q,1}(t) \\ A^+_{k+q,2}(t) \end{array} \right)^T \sigma \cdot [q \otimes k] \left( \begin{array}{c} A_{k,1}(t) \\ A_{k,2}(t) \end{array} \right) \, dk.
\]
Following the procedure outlined above, it is easily verified that the terms of the zeroth order in $\lambda e^2 k$ do not contribute to $\frac{\partial}{\partial t} P(q, t)$. Only the second order term, which is spin dependent, remains

$$
\delta \frac{\partial}{\partial t} \hat{P}(q, t) = i \lambda q \Phi(r, t) \approx \frac{\lambda^2}{2} \int \int V(q) A^*_{\lambda}(s, t) q |q| \sigma |s, s' \rangle A q_{-q, q', t} dQ dq
$$

In configuration representation, averaged over two-component electron Pauli spinors $\Phi(r)$, this contribution leads to the appearance in continuity equation additional material current $\hat{I}_{e,V}(r, t)$ of the form

$$
\hat{I}_{e,V}(r, t) \approx \frac{1}{2} \lambda^2 \frac{\nabla V(r)}{e} \times \Phi(r, t) \sigma \Phi(r, t).
$$

Compare expression for $\hat{I}_{e,V}(r, t)$ with $[8, 11]$. It must be underlined that coincidence with their results occurs only for this expansion, obtained from general one $[64]$ up to the second order in $\lambda e^2 k$. The expressions in the cited papers are valid only within this approximation, while within proposed approach the only constrain is imposed upon is the potential strength. It must be weak enough to create real electron/positron (hole) pairs. One more striking difference lies in the approach to derivation of this term. “Classical” consideration outlined in Landau and Lifshitz textbook $[34]$ is based on variation of applied external fields. The source terms can be represented for classical spin-orbit interaction and Peierls substitution $p \rightarrow p + e/cA(r)$. As it follows from the considerations presented above, the account for vector potential, while deriving this term, is superfluous. This current term is solely due to external potential. Moreover, as in the case of redefinition of probability current under electromagnetic action, we are to expect that different spatial and temporal conditions can be imposed on $\hat{I}_{e,V}(q, t)$ and $\hat{J}_{e}(q, t)$. Such situation (as in superconduction) requires e.g. the stability of bulk state under application of electric field and existence of dissipationless surface currents. Exactly this situation is realized in topological insulators.

V. SUMMARY

We proposed SQM approach for construction of probability and probability current density operators for single particle Pauli-like equation as an alternative to Foldy-Wouthuysen consideration. We partitioned the Hamiltonian (external perturbation accounted for) and operators of interest into the part acting within electron (hole) stationary states and residual part responsible for pair creation/annihilation processes. The effect of residual part is fully neglected in the present paper, assuming that considered external perturbations are weak enough and does not depend on time. The semirelativistic probability and probability current operators, defined within such approximation, demonstrate Gordon-like structure $[18]$, splitting into spin dependent and spin-independent parts. Proposed approach allows to go beyond the commonly used $1/c^2$ approximation. Thus, for example, the defined probability operator predict non-linear dependence on particle momentum for Rashba-like interaction. It was also inferred that in Zeeman term the rest mass in the expression for spin magnetic moment of Pauli electron must be replaced in general by expectation value of energy-dependent Lorentz mass in the corresponding quantum state. The application of external perturbation leads to violation of simple form of continuation equation. It is shown that within proposed approach the continuity equation is valid in general form with sources, dependent on external fields. The source terms can be represented as a divergence of some “material” currents, in full analogy with the description of electromagnetic response in the theory of continuous matter $[8, 11, 53]$.

Based on semi-relativistic similarity of Dirac problem and multicomponent $k \cdot p$ Hamiltonians, we intend to extend the considered approach for the derivation of single quasiparticle probability operators in semiconductors.

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