Singular spin-flip interactions for the 1D Schrödinger operator

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Abstract

We consider singular self-adjoint extensions of one-dimensional Schrödinger operator acting in space of two-component wave functions within the framework of the distribution theory (Kurasov 1996 J. Math. Anal. Appl. 201 297). We show that among \(\mathbb{C}^4\)-parameter set of boundary conditions with state mixing there is only \(\mathbb{R}^2\)-parameter subset compatible with the spin interpretation of the two-component structure of wave function. They can be identified as the point-like spin-momentum (Rashba) interactions. We suggest their physical realizations based on the regularized form of the Hamiltonian with coupling of the electrical field inhomogeneity of a background and spin of a carrier.

Keywords: Schrödinger operator, self-adjoint extensions, spin-momentum coupling, singular interactions, pseudospin

Introduction

Point-like interactions for the Schrödinger operators with inclusion of spin degree of freedom are of great interest for nanotechnology. Spin dependent interactions like the Rashba spin-momentum coupling [1] essentially influence spin dynamics and coherence in materials where such interactions are not small because of specific structure (see [2] and reference therein). In low energy limit when the scale of particle delocalization exceeds all other scales including the range of interaction, one may simplify the interactions considering the point-like potential or inverse scattering length approximation [3–5]. General approach for the description of singular extensions of Hermitian (symmetric) operators is well developed area of operator theory which was initiated by the Faddeev and Berezin paper [6] (see also [5, 7] and the bibliography therein). In particular, singular point-like interactions for the Schrödinger operator

\[
\hat{H}_0 = -\frac{\partial^2}{\partial x^2}.
\]  

form 4-parameter set \(\mathbb{R}^4\) of operators [7, 8]. They all can be derived right from the Dirac operator in one dimension [9, 10]. Besides well known \(\delta\)-potential there are extensions which can be useful for modeling the layered inhomogeneous materials [11–13]. Physical interpretation of these interactions has been proposed in [14, 15]. In this respect spin-dependent interactions can appear as relativistic corrections to classical Hamiltonian (see e.g. [16]). But up to now spin-dependent interactions and their representation within singular perturbation of Hermitian operators have not been thoroughly analyzed from the physical point of view. In the meantime it is clear that taking spin into consideration enriches the number of point-like interactions [17, 18]. For operator equation (1) this is equivalent to consideration of its action in space \(L_2 \otimes L_2\) of two-component wave functions (spinors) and therefore it doubles the number of extensions in comparison with spinless case.

The generalization of known results on the point-like interactions in 1D case onto spin \(s = 1/2\) case using the probability current conservation seems rather straightforward [19]. But it is not necessary to interpret the two-component structure of the wave function in term of spin only since other pseudo-spin interpretations are possible. Indeed, two-component, pseudospin structure of the wave function does not necessary mean the consideration of spin particle. Rather, it is important that the Hamiltonian can be obtained via the reduction of the Dirac-like operator. This brings the concept...
of pseudospin in nuclear physics [20]. In nonrelativistic condensed matter the pseudospin as a rule refers to the spatial degree of freedom and has nothing to do with the intrinsic spin of electrons. The typical example of pseudospin material is graphene [21] where the pseudospin components correspond to the electron wave function on one of the trigonal sublattices. The Dirac cone and the pseudospin is observed in topological insulators as well [22, 23]. The states of particle-hole elementary excitation or layer degree of freedom in a bilayer electron system [24] also give relevant examples of pseudospin-1/2 systems. In contrast to spin case the pseudospin conjugate field may not have direct physical meaning like physical magnetic field which is conjugated to spin degree of freedom. That is why not all extensions allow interpretation as spin dependent interactions. This is one of the point of the paper to derive general matching conditions which do not necessary rely on spin interpretation of multi-component nature of the wave functions. We do it in section 2. Another important issue for physical applications is to obtain the regularized form of the Hamiltonian equation (1) with singular interactions. To do this we use the technique based on the theory of singular perturbations of finite rank for differential operators [7]. This way we derive the corresponding results for spin $s = 1/2$ case as specific example thus demonstrating the consistency with the previously obtained results of [19] in section 3. On this basis in section 4 we show that the point-like interactions of the spin-flip type can be interpreted in terms of spin-momentum (Rashba) interaction pointing the structure of the physical terms which generate spin-flip mechanism through the relativistic spin-momentum interaction in layered 1D systems. We add to the results of [19] the specific analysis of spin operator components involved in interaction and their realization in physical systems. The results are summarized and discussed in Conclusion.

1. Singular interactions for the Schrödinger operator of spinor wave function

The boundary conditions at the singular point for the Hermitian (symmetric) differential operator equation (1) making it self-adjoint operator in $L_2$ can be found easily by imposing the condition of conservation of probability current. In case of 2-component (spinor) wave function the Schrödinger operator equation (1) acts on $L_2 \oplus L_2$

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}.$$  

Then via introducing 4-vector

$$\Gamma = \begin{pmatrix} \psi_1 \\ \psi_1^* \\ \psi_2 \\ \psi_2^* \end{pmatrix}.$$  

the probability current for the Hamiltonian (1)

$$j = 2 \text{Im}(\Psi^* \dot{\Psi}) = 2 \text{Im}(\psi_1^* \dot{\psi}_1 + \psi_2^* \dot{\psi}_2)$$

can be rewritten in the following matrix form:

$$j = \frac{1}{i} \Gamma^\dagger J_4 \Gamma.$$  

Here $J_4$ is the block diagonal $4 \times 4$ skew-symmetric matrix:

$$J_4 = \begin{pmatrix} J_2 & 0 \\ 0 & J_2 \end{pmatrix},$$

where $J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. The skew-symmetric matrix representation of the current equation (4) is due to the fact that self-adjoint boundary conditions are in 1-1 correspondence with the Lagrangian planes (see [25, 26]). Therefore we introduce 4-vector (bispinor) of the boundary values from different sides $x \rightarrow 0 \pm 0$ with respect to the singular point $x = 0$:

$$\Gamma_{0 \pm 0} = \begin{pmatrix} \psi_1 \\ \psi_1^* \\ \psi_2 \\ \psi_2^* \end{pmatrix}_{|0 \pm 0}. $$  

The boundary condition $4 \times 4$-matrix $M$ connects left- and right-hand side values:

$$\Gamma_{0+0} = M \Gamma_{0-0}.$$  

In terms of $M$-matrix the conservation of probability current equation (4) has the form:

$$J_4 = M^\dagger J_0 M,$$

that is $M$ should be a $J_0$-unitary matrix. We consider the extensions (boundary conditions) which depend continuously on the interaction parameters determining the discontinuity values of function and its derivative. We can built the matrices which belong to the connected neighborhood of the unit matrix, i.e. $M = e^X$. From equation (7) we conclude that the generators of the corresponding Lie algebra are determined by the equation:

$$X^\dagger J_4 + J_4 X = 0.$$  

Factorized solutions of equation (8) correspond to non interacting, separable dynamics of wave function components. The BC matrices intertwining the components are:

$$M = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 2z_1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2z_2 \\ -2z_2 \ast & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$  

$$\times \begin{pmatrix} 1 & 0 & 2z_3 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -2z_3 \ast & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 2z_4 \\ 0 & 1 & 0 & 0 \\ 0 & 2z_4 \ast & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$
\[
\begin{pmatrix}
\psi_1' \\
\psi_1 \\
\psi_2 \\
\psi_2' \\
\end{pmatrix}
= 
\begin{pmatrix}
\psi_1' + 2z_1 \psi_2 \\
\psi_1 + 2z_2 \psi_2' \\
\psi_2 + 2z_1^* \psi_1' \\
\psi_2' + 2z_2^* \psi_1 \\
\end{pmatrix}
\]  
\times 
\begin{pmatrix}
\psi_1 + 2z_2 \psi_2 \\
\psi_1' + 2z_2 \psi_2' \\
\psi_2' - 2z_2^* \psi_1' \\
\psi_2 - 2z_2^* \psi_1 \\
\end{pmatrix}
\]  
(10)

with \(z_i \in \mathbb{C}\) so we have \(C^4\) set of extensions of point-like interactions with the exchange between components of state vector \(\Psi\). Note that here we are not restricted by the spin interpretation and can interpret the two-component nature of state vector within the pseudospin picture which broads the application range.

### 1.1. Singular distribution approach

The basic representation of the singular interactions of the Schrödinger operator of a free particle in one dimension was given by Kurasov in [8] (see also [7]). In simple terms the result is that for the operator equation (1) all possible BC’s at the singular point describe the jumps in wave function and its derivative. So one comes to the consideration of the functionals on the space of bounded functions and their derivatives outside the singular point \((x = 0)\) with possible discontinuity at the singular point. Here we adjust the general theory of [7] to the case of the Schrödinger operator which acts in the Hilbert space of 2-component wave equation (2).

Following the general scheme of [7] we define the following distributions for the components:

\[
\delta_i[\Psi] = \frac{\psi_i(0-) + \psi_i(0+)}{2}, \\
\delta_i^{(1)}[\Psi] = -\frac{\psi_i'(0-) + \psi_i'(0+)}{2}, \\
\beta_i[\Psi] = \frac{\psi_i(0+) - \psi_i(0-)}{2}, \\
\beta_i^{(1)}[\Psi] = -\frac{\psi_i'(0+) - \psi_i'(0-)}{2}
\]

and introduce the vector-functionals

\[
\Delta_i = \left(\delta_i, \delta_i^{(1)}\right)
\]

Then the operator expression

\[
\hat{H}_t = \begin{pmatrix}
-D_1^2 & 0 \\
0 & -D_1^2
\end{pmatrix} + \begin{pmatrix}
\Delta_1^T \Delta_1 & \Delta_2^T \Delta_2 \\
\Delta_1^T \Delta_2 & \Delta_2^T \Delta_1
\end{pmatrix}
\]

(13)

determines the Hamiltonian of a free particle augmented with the point-like interactions. Equation (13) defines a finite rank perturbation of the Schrödinger operator (see formal definitions of corresponding functional spaces in [7]). The second term in equation (13) is the Hermitian quadratic form of linear functionals. The matrices \(h_{ij}\) of size \(2 \times 2\) form the

Hermitian block matrix:

\[
\mathbf{h} = \begin{pmatrix}
h_1^1 & h_1^2 \\
h_2^1 & h_2^2
\end{pmatrix}
\]

(14)

The relation between matrices \(\mathbf{h}\) and the boundary value matrices \(\mathbf{M}\) can be found using the general theory [7] and is as following:

\[
\mathbf{M} = (1 + J_4 \mathbf{h})(1 - J_4 \mathbf{h})^{-1}.
\]

(15)

So using equation (15) we find that the BC matrices equation (9) with state mixing correspond to the following singular interaction matrices in equation (13):

\[
\mathbf{h} = \begin{pmatrix}
0 & 0 & -z_1 & 0 \\
0 & 0 & 0 & 0 \\
-z_1^* & 0 & 0 & 0 \\
0 & 0 & 0 & -z_2^*
\end{pmatrix}
\]

\times \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & z_3 & 0 \\
0 & z_3^* & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]

(16)

In the following section we build the regularized form of the singular Hamiltonian equation (13). Such a form is useful for physical realization of point-like interactions which are nothing but limiting cases of spatial inhomogeneities of specific physical fields [19].

### 2. Regularized form of point-like interactions

Basing on the results of previous section and applying technique of [8] we can give explicit regularized form of the Hamiltonian. Let us define the linear space \(K\) of test functions which are continuous and bounded along with their derivatives outside \(0\) (see details of formal definitions in [7, 8]). Let \(K\) is the dual linear space i.e. the linear space of distributions on \(K\). In two-component case we consider the differential operator

\[
\hat{H}_t = \begin{pmatrix}
H_{1,1} & H_{1,2} \\
H_{2,1} & H_{2,2}
\end{pmatrix}
\]

(17)

which can be represented as the following:

\[
\hat{H}_t = (i D_2)^2 \begin{pmatrix}
1 + a_{1,1} \Delta_{1,1} & a_{1,2} \Delta_{1,2} \\
a_{2,1} \Delta_{2,1} & 1 + a_{2,2} \Delta_{2,2}
\end{pmatrix}
\]

\[
+ \begin{pmatrix}
b_{1,1} \Delta_{1,1} & b_{1,2} \Delta_{1,2} \\
b_{2,1} \Delta_{2,1} & b_{2,2} \Delta_{2,2}
\end{pmatrix}
\]

\[
+ \begin{pmatrix}
c_{1,1} \Delta_{1,1} & c_{1,2} \Delta_{1,2} \\
c_{2,1} \Delta_{2,1} & c_{2,2} \Delta_{2,2}
\end{pmatrix}
\]

(18)

where vectors \(\mathbf{a}, \mathbf{b}, \mathbf{c}\) determine the parameters of corresponding singular interactions. This operator acts on the corresponding Sobolev space \(W^2_2(\mathbb{R}\setminus 0) \oplus W^2_2(\mathbb{R}\setminus 0)\) and maps it into linear space of functionals \(K' \oplus K'\) due to
actions of the following operators
\[ \Delta_{ij} = \begin{pmatrix} \delta_{ij} \\ \delta_{1j} \end{pmatrix}. \]  

(19)

Then the product of \( \delta \)-distribution and its derivative (the elements of \( K \)) and the elements \( \psi \in K \) can be written as:
\[ \delta_{ij} \psi = \delta_i[\psi] \delta_j + \beta_i[\psi] \beta_j \]  

(20)

\[ \delta_{ij}^{(2)} \psi = \delta_i^{(1)}[\psi] \delta_j + \beta_i^{(1)}[\psi] \beta_j + \delta_i[\psi] \delta_j^{(1)} + \beta_i[\psi] \beta_j^{(1)} \]  

(21)

which are analogs to the expressions of scalar case (see [7, 8]). Being restricted to the subspace of continuous functions equation (18) maps it onto 4-dim subspace of distributions spanned by the functionals \( \delta_k^i, k = 0, 1, 2, 3 \). Imposing the constraint \( L \Psi \in L_2 \bigoplus L_2 \) we get the relations
\[
\begin{pmatrix}
-a^{(1)}_{1,1} & 0 & 0 & 0 & -a^{(1)}_{1,2} & 0 & 0 & 0 \\
-b^{(0)}_{1,1} - a^{(1)}_{0,1} & 0 & 0 & 0 & b^{(1)}_{1,1} - a^{(1)}_{0,1} - a^{(1)}_{2,1} & 0 & 0 \\
-b^{(0)}_{1,1} + c^{(1)}_{1,1} & 0 & 0 & 0 & b^{(0)}_{1,1} + c^{(1)}_{1,1} - a^{(1)}_{2,2} & 0 & 0 \\
-a^{(1)}_{2,2} & 0 & 0 & 0 & -a^{(1)}_{2,2} & 0 & 0 & 0 \\
-b^{(0)}_{2,1} - a^{(1)}_{0,2} & 0 & 0 & 0 & b^{(1)}_{2,1} - a^{(1)}_{0,2} - a^{(1)}_{1,2} & 0 & 0 \\
-b^{(0)}_{2,1} + c^{(1)}_{2,1} & 0 & 0 & 0 & b^{(0)}_{2,1} + c^{(1)}_{2,1} - a^{(1)}_{1,2} & 0 & 0 \\
-c^{(0)}_{2,1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
c^{(0)}_{2,1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
\delta_i[\psi] \\
\delta_{1i}^{(1)}[\psi] \\
\beta_i[\psi] \\
\beta_{1i}^{(1)}[\psi] \\
\delta_i^{(1)}[\psi] \\
\beta_{i}^{(2)}[\psi] \\
\beta_{i}^{(3)}[\psi] \\
\beta_{i}^{(4)}[\psi] \\
\end{pmatrix}
\]

(22)

\[ = 0. \]

The boundary conditions follow from the demand that the rank of the matrix in equation (22) is equal to 4. Therefore we get:
\[ a^{(1)}_{1,1} = 0, \quad i b^{(1)}_{1,1} = a^{(0)}_{1,1}, \quad a^{(1)}_{1,2} = 0, \quad i b^{(1)}_{2,1} = a^{(0)}_{1,2} \]  

(23)

\[ a^{(1)}_{2,1} = 0, \quad i b^{(1)}_{2,1} = a^{(0)}_{2,1}, \quad a^{(1)}_{2,2} = 0, \quad i b^{(1)}_{2,2} = a^{(0)}_{2,2} \]  

(24)

and the corresponding BC’s are:
\[
\begin{pmatrix}
-\delta_{1i}^{(1)}[\psi] \\
\beta_{1i}^{(1)}[\psi] \\
\delta_{2i}^{(1)}[\psi] \\
\beta_{2i}^{(2)}[\psi] \\
\beta_{2i}^{(3)}[\psi] \\
\beta_{2i}^{(4)}[\psi] \\
\end{pmatrix} = \Lambda \begin{pmatrix}
\delta_i[\psi] \\
\delta_{1i}^{(1)}[\psi] \\
\beta_i[\psi] \\
\beta_{1i}^{(1)}[\psi] \\
\delta_i^{(1)}[\psi] \\
\beta_{i}^{(2)}[\psi] \\
\beta_{i}^{(3)}[\psi] \\
\beta_{i}^{(4)}[\psi] \\
\end{pmatrix}, \]  

(25)

where
\[ \Lambda = \begin{pmatrix}
ib^{(0)}_{1,1} + c^{(1)}_{1,1} & ib^{(1)}_{1,1} & ib^{(0)}_{1,2} + c^{(1)}_{1,2} & ib^{(1)}_{1,2} \\
-c_{1,1}^{(0)} & -c_{1,1}^{(0)} & -c_{1,2}^{(0)} & -c_{1,2}^{(0)} \\
ib^{(0)}_{2,1} + c^{(1)}_{2,1} & ib^{(1)}_{2,1} & ib^{(0)}_{2,2} + c^{(1)}_{2,2} & ib^{(1)}_{2,2} \\
-c_{2,1}^{(0)} & -c_{2,1}^{(0)} & -c_{2,2}^{(0)} & -c_{2,2}^{(0)} \\
\end{pmatrix}. \]  

(26)

As long as we are interested in spin-flip BC’s only we may put diagonal coefficients to zero so that equation (25) becomes as following:
\[
2 \begin{pmatrix}
\beta_i[\psi] \\
\beta_{1i}^{(1)}[\psi] \\
\beta_{2i}^{(2)}[\psi] \\
\beta_{2i}^{(3)}[\psi] \\
\end{pmatrix} = \begin{pmatrix}
0 & 0 & ib^{(0)}_{1,2} + c^{(1)}_{1,2} & ib^{(1)}_{1,2} \\
0 & 0 & -c^{(0)}_{1,2} & -c^{(0)}_{1,2} \\
ib^{(0)}_{2,1} + c^{(1)}_{2,1} & ib^{(1)}_{2,1} & 0 & 0 \\
-c^{(0)}_{2,1} & -c^{(0)}_{2,1} & 0 & 0 \\
\end{pmatrix} \begin{pmatrix}
\delta_i[\psi] \\
\delta_{1i}^{(1)}[\psi] \\
\beta_i[\psi] \\
\beta_{i}^{(2)}[\psi] \\
\end{pmatrix} \]  

(27)

The current conservation equation (4) imposes additional constraints:
\[ c^{(0)}_{2,1} = c^{(1)}_{2,1}, \quad c^{(1)}_{2,1} = c^{(1)}_{1,2} + i b^{(0)}_{1,2}, \quad b^{(1)}_{2,1} = -b^{(1)}_{1,2}, \quad b^{(0)}_{2,1} = b^{(0)}_{1,2}. \]  

(28)

Let us denote:
\[ z_1 = -c^{(0)}_{1,2}, \quad z_2 = c^{(1)}_{1,2}, \quad z_3 = -c^{(1)}_{1,2}, \quad z_4 = a^{(0)}_{1,2}, \quad z_i \in \mathbb{C}. \]  

(22)

From equations (27), (28) we finally obtain \( \mathbb{C}^4 \) set of spin-flip BC’s matrices:
\[ \Lambda = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & z_1 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix} \begin{pmatrix}
0 & 0 & z_2 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & z_3 & 0 \\
\end{pmatrix} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix}. \]  

(29)

On the other hand, according to [7] the matrix \( \Lambda \) can be represented as \( \Lambda = J_0 \mathbf{h} \) so that equation (29) leads exactly to equation (9). As long as operator with singular interaction equation (18) can be approximated by the second order differential operators with smooth coefficients the Hamiltonian has the following regularized form
\[ \hat{H}_s = (i D_y) \begin{pmatrix} 1 & z_4 \delta \varepsilon \\ z_4^* \delta \varepsilon & 1 \end{pmatrix} (i D_y) + (i D_x) \begin{pmatrix} 0 & -i(z_2 + z_3) \delta \varepsilon \\ i(z_2^* + z_3^*) \delta \varepsilon & 0 \end{pmatrix} + \begin{pmatrix} 0 & -z_4 \delta \varepsilon - z_3 \delta \varepsilon^{(1)} \\ -z_4^* \delta \varepsilon + z_3^* \delta \varepsilon^{(1)} & 0 \end{pmatrix}, \]

where \( \delta \varepsilon, \delta \varepsilon^{(1)} \) are smooth and even \( \varepsilon \)-approximands of the corresponding functionals. They represent spatial inhomogeneities of physical fields.

Other solutions represent the BC’s without state mixing and correspond to known cases [5, 8] for each of the components. We will not consider them thoroughly and just give one example of relevant physical situation which could be of interest in this case.

Having established the BC’s in 1 dimension we can apply these results to 3D case. The latter can be effectively reduced to one dimensional problem on semi-axis \( r > 0 \) with \( \phi(r) = r \psi(r) \) as the effective 1D wave function through the natural definition domain of free Hamiltonian:

\[ ||\hat{H}_0 \psi||_2^2 = \int_0^\infty |(r \psi)(r)|^2 \mathrm{d} r < \infty. \]  

Then the limiting value \( \phi(0) \) as well as its derivative \( \phi'(0) \) is defined since equation (31) is well defined on the corresponding Sobolev space \( W^2_2(\mathbb{R}_+) \) which is dense in \( L_2(\mathbb{R}_+) \). The conservation of the probability current:

\[ J = \int_0^\infty \text{Im} \left( \Psi \frac{\partial \Psi}{\partial r} \right)^2 \mathrm{d} r = \int_0^\infty \text{Im} \left( r \Psi \frac{\partial (r \Psi)}{\partial r} \right) \mathrm{d} r \]

leads to the BC’s of the following form:

\[ \Phi' = W \Phi, \]

where \( W \) is the hermit an matrix and:

\[ \Phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad \Phi' = \begin{pmatrix} \phi'_1 \\ \phi'_2 \end{pmatrix} \]

are 2-spinor boundary-value vectors. The standard representation:

\[ W = \Omega 1 + \mathbf{w} \cdot \mathbf{\sigma}, \]

where \( \sigma \) is the Pauli matrices vector allows to identify the scalar part (first term) as the standard point-like potential b.c. [3, 6]:

\[ \Phi' = \Omega \Phi \]

independent on the spin state. The vector part (traceless second term) of equation (35) describes polarizational contact interactions. Namely spin-dependent version of equation (36) is:

\[ \Phi' = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Phi, \]

where the bound state exists only for one component (e.g. for \( \downarrow \)-state if \( \omega > 0 \) ). Combining this case with the standard ZRP equation (36) with \( \Omega < 0, |\Omega| > |\omega| \) it is possible to get two bound states with

\[ E_{1,\downarrow} \sim - (\Omega \pm \omega)^2 \]

for \( \uparrow \downarrow \) - states. Thus equation (38) can be treated as the hyperfine splitting due to Fermi contact interaction [27] between the magnetic moments of an ‘electron’ and a ‘nucleus’, i.e. the singular center.

For the physical analysis of different singular terms in equation (30) we can apply the results obtained for spinless case in [15]. It allows to suggest that \( z_2 \) and \( z_4 \) couplings are caused by different inhomogeneities of the effective mass operator spatial profile. The couplings \( z_1 \) and \( z_3 \) are due to ‘scalar’ and ‘vector’ part of the external potential correspondingly augmented with the component mixing. For complete understanding of physical nature of these interactions one need to specify the physical nature of the wave function components to distinguish between spin and pseudospin interpretations.

3. Spin-motion (Rashba) point-like interactions

Spin interpretation of two-component state vector \( |\psi\rangle \) implies additional constraint on the structure of probability current. In fact in such physical situation we deal with the Pauli Hamiltonian:

\[\hat{H} = \left( \frac{\hat{p} - q}{\hbar} \mathbf{A} \right)^2 + q \varphi - \frac{q}{\hbar} \mathbf{\sigma} \cdot \vec{H}, \]

where \( \mathbf{\sigma} \) representing the vector of Pauli matrices and \( \vec{H} \) is the magnetic field with \( \mathbf{A} \) as its vector potential and \( \varphi \) being the scalar potential. The probability current for (39) is as following:

\[ J_y = \frac{\hbar}{m} \text{Im} \left( \Psi \nabla \Psi ^* \right) - \frac{q}{mc} \mathbf{A} \Psi \Psi ^* + \frac{\hbar}{2m} \text{rot} (\Psi \mathbf{\sigma} \Psi ^*), \]

where the last term is due to the magnetization current (see e.g. [16]). The constraint of conservation of equation (40) reduces the number of BC’s with the spin-flip to only two-parameter set \( \mathbb{R}^2 \) because of the conservation constraints for \( y, z \) components of (40) (see details in [19]):

\[ J_y = - \left( \frac{\partial \Psi}{\partial x} \mathbf{\sigma} \Psi + \Psi \frac{\partial \Psi}{\partial x} \mathbf{\sigma} \right), \]

\[ J_z = \frac{\partial \Psi}{\partial x} \mathbf{\sigma} \Psi + \Psi \frac{\partial \Psi}{\partial x} \mathbf{\sigma}. \]

Namely, there are only two self-adjoint b.c.’s:

\[ \mathbb{M}^{(r)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 2 X_4^{(r)} & 0 & 0 & 1 \end{pmatrix}, \]

which mix the spin components of the wave function. In [19] it was suggested that b.c.’s equation (43) can be considered as
point-like spin-momentum interactions (Rashba couplings). Here we demonstrate the same result directly basing on the structure of the Hamiltonian equation (30). First we need to specify the spin operator for which the components \( \psi'_{1,2} \) are eigenstates. Since \( x \)-axis is the only spatial inhomogeneity and the structure of the spin interaction terms is given by the relativistic spin-momentum (Rashba) coupling (see [16, 28]):

\[
\hat{H}_{\text{int}} = \lambda (\nabla \varphi \times \mathbf{p}) \cdot \hat{S}
\]

(44)

therefore \( y, z \)-components of the spin operator are the only ones involved in equation (44). Let us consider the simplest specific example of \( \delta \)-interaction with the spin-flip (\( z_1 \)-coupling). Taking into account the cyclic property of the Pauli matrices and using the representation

\[
\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}
\]

we see that the only consistent choice is to treat \( \psi_{1,2} \) as the eigenstates of \( \hat{S}_z \) operator. In regularized form using the spin representation for equation (30):

\[
\hat{H}_{z_1} = (i D_y)^2 + (a \sigma_y + b \sigma_z) \delta_z(x),
\]

\[
a \sim \text{Re} \ z_1, \quad b \sim \text{Im} \ z_1.
\]

(45)

Comparing it with equation (43) we get \( b = 0 \). The same reasoning works for \( z_2 \)-coupling. Therefore we get the Hamiltonian with the singular spin-flip interactions:

\[
\hat{H}_{z_2} = (i D_y) (i + X_4^{(r)} \sigma_y) \delta (i D_y) + X_4^{(i)} \sigma_y \delta
\]

(46)

with

\[
X_4^{(r)} = - \text{Re} \ z_2, \quad X_4^{(i)} = - \text{Re} \ z_4.
\]

Substituting these results in equation (10) we get the following BC’s:

\[
\begin{pmatrix}
\psi_1 \\
\psi'_1 \\
\psi_1 \\
\psi'_1
\end{pmatrix}_{0+0} = 
\begin{pmatrix}
\psi_1 \\
\psi'_1 + 2 X_4^{(r)} \psi'_1 \\
\psi_1 \\
\psi'_1 + 2 X_4^{(i)} \psi'_1
\end{pmatrix}_{0-0}.
\]

(47)

\[
\begin{pmatrix}
\psi_1 \\
\psi'_1 \\
\psi_1 \\
\psi'_1
\end{pmatrix}_{0+0} = 
\begin{pmatrix}
\psi_1 \\
\psi'_1 + 2 X_4^{(r)} \psi'_1 \\
\psi_1 \\
\psi'_1 + 2 X_4^{(i)} \psi'_1
\end{pmatrix}_{0-0}.
\]

(48)

They coincide with those obtained in [19]. Thus the regularized form of the spin-flip Hamiltonian is:

\[
\hat{H} = (i D_y) (i + X_4^{(r)} \sigma_y) \delta_z(x) (i D_y) + X_4^{(i)} \sigma_y \delta_z(x)
\]

(49)

which means that the spin projections \( S_i = \frac{h}{2} \sigma_i, i = x, z \) are not integrals of motions anymore.

Thus the interpretation of two-component nature of \( \Psi \) as spin degree of freedom singles 2-parameter set \( \mathbb{R}^2 \) out of the set \( \mathbb{C}^4 \) of possible extensions equation (16). As is clear from the structure of equation (49) we may attribute \( X_4^{(r)} \)-coupling to the Rashba interaction of the ‘bare’ carrier due to the inhomogeneous electrostatic field and transverse component of the momentum \( p_z \). The same is true for \( X_4^{(i)} \)-coupling though in this case such field modifies the kinetic energy term. We may conclude that this is due to spatial dependent effective mass. Thus the BC corresponding to this singular extension can be realized in systems where the propagation of a particle in a medium lead to its ‘dressing’ and dynamic contribution to the mass operator. The latter thus expected in the materials with spatially variable effective mass of the carriers. As to the pseudospin case the realization of singular interactions in terms of physical fields depends on the specific nature of pseudospin degree of freedom.

**Conclusion**

In this paper we have reproduced the results of [19] on point-like interactions for the Schrödinger operator equation (1) on space of two-component wave functions \( L_2 \oplus L_2 \). We use the Kurusov’s technique for construction of singular perturbations of self-adjoint operators [7] and show that there is \( \mathbb{C}^4 \) set of singular interactions with interstate mixing equation (16). If one uses spin interpretation of two-component wave vector then this set reduces to \( \mathbb{R}^2 \) i.e. only two spin-momentum couplings equations (47), (48). The coupling equation (47) is due to localized inhomogeneity of the potential barrier. Boundary conditions (48) can be expected in systems where the effective mass spatial profile has essentially non monotonous character as we can conclude heuristically from the results of [15] obtained for spinless particle. Yet rigorous treatment is needed in order to extend the result of [11] onto spin \( s = 1/2 \) case. Besides spin-dependent point-like interactions can be realized as the thin magnetized interface in layered system. From such a point of view it is important to analyze extensions for Aharonov–Bohm Hamiltonian in 2D [17, 29]. Here one can expect interesting interplay between localized magnetic flux (see [18]) and relativistic spin-momentum interactions [29, 30] which is of interest for studying low dimensional magnetic systems. It seems that the spin-flip self-adjoint extensions which represent point-like spin-momentum coupling can be also obtained by the standard von Neumann method for the Dirac Hamiltonian similar to that used in [9, 10, 31, 32] as the spin dependent interactions were not considered there. Since such (pseudo)spin-momentum coupling breaks the spherical symmetry of the Hamiltonian it is natural to consider the influence of spin \( s = 1/2 \) degree of freedom on spherically symmetrical \( \hat{V}(r) = a \delta(r - r_0) + b \delta'(r - r_0) \) point-like interactions [33] confined to hyperspheres. The nature of other one dimensional b.e.’s in deals with the pseudospin interpretations of two-component nature of the wave function, e.g. particle-hole excitation states near Fermi level or wave function amplitudes on some substructures. In fact, any two-component quantum degree of freedom of the carrier with \( U(2) \)-symmetry can be treated mathematically equivalent to spin, and can therefore be called a pseudospin. For such degree of freedom corresponding pseudospinorbit coupling and an effective magnetic field can be also introduced depending on its physical realization [24]. With this one can search for new effects characteristic for spectral properties of pseudospin...
Hamiltonian for the chains of singular interactions with respect to interaction strength disorder [23, 34] or nonuniform placement of the singular centers with limiting points [35].

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