NON-MINIMAL INTERACTION AND SPECTRA OF IMPURITY STATES FOR LIGHT CARRIERS IN KANE'S SEMICONDUCTORS

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The energy spectrum of impurity states is calculated for Coulomb potential in Kane's type semiconductors using non-minimal interaction way.

The solutions of Dirac equations with minimal and non-minimal interactions terms were investigated in [1-4] by transforming relativistic equation into the Schrodinger like equation. It was shown [1] that if one makes a non-minimal replacement

$$\vec{p} \rightarrow \vec{p} - i\beta m\omega\vec{r} \tag{1}$$

in Dirac equation, where β is a diagonal matrix with elements ± 1, it can be transformed into the Schrodinger oscillator equation with parabolic potential and additional constant term the nature of which is connected with spin-orbital interaction.

It was shown in [5] that in the case of Kane's equation the non-minimal substitution of the form (1) also leads to the Schrodinger equation with harmonic oscillator potential. Other examples of non-minimal substitutions were considered in [6-7]. Non-minimal substitution of the form

$$\vec{p} \rightarrow \vec{p} - i\beta\frac{\vec{r}}{r} \tag{2}$$

in the Dirac equation leads to the Schrodinger equation with Coulomb potential. In this paper the same investigation was carried out for the Kane's equation describing the spectra of the electrons, light and heavy holes, and the spin-orbit splitting valence bands for the A^3B^5 type (InSb, InAs, GaAs and etc.) semiconductors. In the eight-band Kane's Hamiltonian the valence and conduction bands interaction are taken into account via the only matrix element P (so called Kane's parameter). The sistem of the Kane's equations including the nondispersional heavy holes band has a form [8-9]:

$$(\alpha\cdot k\cdot P + \beta\cdot G - E)\Psi = 0 \tag{3}$$

где

$$\alpha_x = \begin{pmatrix} 0 & 0 & \frac{-1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} \\ 0 & 0 & 0 & \frac{-1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & 0 \\ \frac{-1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{4}$$

$$\alpha_y = \begin{pmatrix} 0 & 0 & \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{6}} & 0 & 0 & \frac{i}{\sqrt{3}} \\ 0 & 0 & 0 & \frac{i}{\sqrt{6}} & 0 & \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{3}} & 0 \\ \frac{-i}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-i}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{-i}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-i}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{-i}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{5}$$

$$\alpha_z = \begin{pmatrix} 0 & 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & \sqrt{\frac{1}{3}} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & -\sqrt{\frac{1}{3}} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{2}{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{2}{3}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{1}{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{\frac{1}{3}} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{6}$$

$$G = \begin{pmatrix} E_g & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_g & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_g+\Delta & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_g+\Delta \end{pmatrix} \tag{7}$$

$$\beta=\begin{pmatrix}1&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&-1&0&0&0&0&0\\0&0&0&-1&0&0&0&0\\0&0&0&0&-1&0&0&0\\0&0&0&0&0&-1&0&0\\0&0&0&0&0&0&-1&0\\0&0&0&0&0&0&0&-1\end{pmatrix} \quad (8),$$

$$\Psi=\begin{pmatrix}\Psi_1\\\Psi_2\\\Psi_3\\\Psi_4\\\Psi_5\\\Psi_6\\\Psi_7\\\Psi_8\end{pmatrix} \quad (9)$$

E_g is a band gap energy, Δ is a value of spin-orbital splitting and

$$k=-i\nabla \quad (10)$$

We substitute

$$\vec{k}\to\vec{k}-i\lambda\beta\frac{\vec{r}}{r}, \quad (11)$$

in Kane's system of equations. Expressing all components of the wave function by the first two we obtain:

$$\left(A-\frac{B}{r\hbar}L_z\right)\Psi_1-\frac{B}{r\hbar}L_+\Psi_2=0 \quad (12)$$

$$\left(A+\frac{B}{r\hbar}L_z\right)\Psi_2-\frac{B}{r\hbar}L_-\Psi_1=0 \quad (13)$$

где

$$A=E_g-E+\frac{P^2(3E+2\Delta)}{3(\Delta+E)E}\left(-\nabla^2+\lambda^2+\frac{2\lambda}{r}\right),$$
$$B=\frac{2}{3}\frac{P^2\Delta\lambda}{E(\Delta+E)} \quad (14)$$

$$L_\pm=L_x\pm iL_y,$$

L_x, L_y, L_z are angular momentum operator components. The spherical symmetry of this problem gives the possibility to express the solution of the differential equation in the form $F(r)Y(\theta,\varphi)$. Acting on the equation (13) with an operator L_- and using the commutative relations for operators $L_\pm$, L_z we obtain the expressions for $L_-\psi_2$. The substitution of the obtained value for $L_-\psi_2$ into the equation (12) gives two equations for $F(r)$:

$$\left(A-\frac{B}{2r}\mp\frac{B}{r}\left(l+\frac{1}{2}\right)\right)F(r)=0 \quad (15)$$

After substituti on of the values of A and B from (14) the equation (15) can be rewritten in the form:

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}+\frac{2m_n}{\hbar^2}\left(E'+\frac{N}{r}\right)\right)F(r)=0 \quad (16)$$

where

$$E'=\frac{E(E-E_g)(E+\Delta)}{3E+2\Delta}\cdot\frac{3}{P^2}\frac{\hbar^2}{2m_n}-\frac{\hbar^2\lambda^2}{2m_n} \quad (17)$$

$$N=-\frac{\hbar^2\lambda}{m_n}\left(1-\frac{\Delta}{3E+2\Delta}\left(\frac{1}{2}\pm\left(l+\frac{1}{2}\right)\right)\right) \quad (18)$$

The solution of (16) reads [13]:

$$F(\rho)=\rho^l\exp\left(-\frac{\rho}{2}\right)F(-n+l+1;2l+2;\rho), \quad (19)$$

$F(-n+l+1,\ 2l+2,\ \rho)$ is a confluent hypergeometric function, $n-l-1=p$ must be positive integer or zero and

$$\rho=\frac{2}{\hbar}\sqrt{-\frac{2m_nE'}{\hbar}}\,r \quad (20)$$

The energy spectrum is determined by an expression:

$$E'=-\frac{N^2}{2\hbar^2}\frac{m_n}{n^2} \quad (21)$$

The Kane's parameter P is connected with effective mass m_n in a usual way:

$$P^2=\frac{3\hbar^2}{2m_n}\frac{E_g(E_g+\Delta)}{3E_g+2\Delta} \quad (22)$$

Substituting the values of E', N, and P consequently from equations (17), (18) and (22) into (21) one can obtain the equation:

$$\frac{E(E-E_g)(E+\Delta)}{3E+2\Delta}\cdot\frac{3E_g+2\Delta}{E_g(E_g+\Delta)}-\frac{\hbar^2\lambda^2}{2m_n}=-\frac{\hbar^2\lambda^2}{2m_nn^2}\left(1-\frac{\Delta}{3E+2\Delta}\left(\frac{1}{2}\pm\left(l+\frac{1}{2}\right)\right)\right)^2\frac{1}{n^2} \quad (23)$$

It is seen from (23) that the energy of impurity states depends on two quantum numbers n and l. This means that the degeneration on quantum number l is removed. Let us consider two limiting cases.

The first, when spin-orbital splitting is small in comparison with the energy gap ($\Delta<<E_g$), takes place in all GaAs type wide band semiconductors. Then the equation (23) can be reduced to the form:

$$\frac{E(E-E_g)}{E_g}=\frac{\hbar^2\lambda^2}{2m_n}\left(1-\frac{1}{n^2}\right) \tag{24}$$

For shallow acceptor states ($E>0$, $E<<E_g$) it can be obtained from (24):

$$E=-\frac{\hbar^2\lambda^2}{2m_n}+\frac{\hbar^2\lambda^2}{2m_n}\frac{1}{n^2} \tag{25}$$

It is seen from (25) that the impurity states is connected with light carriers and has hydrogen-like spectrum. If one choose the value of λ in (11) in the form $\lambda=\frac{Ze^2m_n}{\chi\hbar^2}$ where χ is the static dielectric constant of the medium and Ze is the charge of the center then the equation (25) turns into the solution of the Shrodinger equation with the Coulomb potential shifted by $(Z^2e^4m_n/2\chi^2\hbar^2)$. Further we shall not consider this constant term in (25).

The equation (24) takes into account the non parabolicity of light carriers spectra too.

The second, when spin-orbital splitting is strong ($\Delta>>E_g$), which takes place in InSb or InAs. In this case the equation (23) transforms in to the form:

$$\frac{E(E-E_g)}{E_g}=-\frac{Z^2e^4m_n}{2\chi^2\hbar^2}\left(1-\frac{1}{2}\left(\frac{1}{2}\pm\left(l+\frac{1}{2}\right)\right)\right)^2 \tag{26}$$

It is easy to obtain from (26) for the acceptor states ($E>0$, $E<<E_g$):

$$E_{\mp}=\frac{Z^2e^4m_n}{2\chi^2\hbar^2}\frac{(3\mp(2l+1))^2}{16}\frac{1}{n^2} \tag{27}$$

The ground state energy ($n=1$, $l=0$) reads:

$$E_+=\frac{Z^2e^4m_n}{2\chi^2\hbar^2} \tag{28}$$

Spectrum of donor states, which are placed below the E_g, can be obtained by the same way.

The problem of impurity states in Kane's type semiconductors, when Coulomb potential have been introduced into the Shroedinger equation by a standard way through the scalar potential was considered in [10-12]. As it was shown in these works there are two types of acceptor states in GaAs type crystals, connected with the valence bands. The first type states are connected with the heavy holes zone and described by the hydrogen-like spectrum. The second type states are due to the zone of light carriers and are described by the Dirac type spectrum. In InSb-type crystals the impurity states always are of Dirac-type.

We have shown in this paper that if one introduces Coulomb potential by non-minimal way then in Kane's model two types of solution are obtained depending on the value of spin orbital-splitting. For $E<<E_g$ we have the usual hydrogen like spectrum as for donor and as for acceptor states, the last being connected with the zone of light holes only. In the case when ($\Delta>>E_g$ the degeneration in orbital quantum number l is removed. However, in both cases the ground state energy have the form corresponding to the solution of the standard Shrodinger equation with Coulomb potential. This result is in accordance with the obtained earlier solutions for Kane's Hamiltonian which describes the spectrum of light charged carriers [10,11].

The author thanks F.M. Gashimzade and O.Z. Alekperov, for the useful remarks and discussion of results and E.Djafarov for attraction of his attention to works [6,7].

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QEYRİ-MİNİMAL QARŞILIQLI TƏSİR VƏ KEYN TİPLİ YARIMKEÇİRİCİLƏRDƏ YÜNGÜL YÜKDAŞIYICILARIN AŞQAR HALLARININ ENERJİ SPEKTRLƏRİ

Keyn tipli yarımkeçiricilərdə Kulon potensialı üçün aşqar halların enerji spektrləri qeyri-minimal qarşılıqlı təsir metodu ilə hesablanmışdır.

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НЕМИНИМАЛЬНОЕ ВЗАИМОДЕЙСТВИЕ И СПЕКТР ПРИМЕСНЫХ СОСТОЯНИЙ ЛЕГКИХ НОСИТЕЛЕЙ ЗАРЯДА В КЕЙНОВСКИХ ПОЛУПРОВОДНИКАХ

Методом неминимального взаимодействия рассчитан энергетический спектр примесных состояний, связанных с кулоновским потенциалом в кейновских полупроводниках.

Received: 10.12.02