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DIAGONAL AND NONDIAGONAL MATRIX ELEMENTS OF THE EFFECTIVE HAMILTONIAN OF ELECTRONS IN A SEMICONDUCTOR (TAKING INTO ACCOUNT SPIN-ORBIT INTERACTION)

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ABSTRACT

The matrix elements of the effective Hamiltonian of current carriers are calculated as in the Kane approximation, where the conduction band, the valence band consisting of light and heavy hole subbands, and the spin-split band, as well as in the Luttinger-Kohn model, are considered.

KEYWORDS: ***matrix element, effective Hamiltonian, current carriers, wave function.***

INTRODUCTION

It is known that many physical parameters of the crystalline potential depend on the band structure of the semiconductor [1-5]. Moreover, usually in band theory it is believed that the crystalline periodic potential is always an even function of coordinates. However, in some cases, for example, in a semiconductor, where there is a heterojunction, the periodic potential of the crystal, along with the symmetric part, can have an asymmetric part.

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THE MAIN RELATIONSHIPS

This case requires a separate analysis of the matrix elements of the effective Hamiltonian of current carriers as in the Kane approximation, where the conduction band, the valence band consisting of light and heavy hole subbands, and the spin-split band, as well as in the Luttinger-Kohn model [6, 7]. Next, we consider the case when the extreme points of the zones are in the center of the Brillouin zone, i.e. at the point $\vec{k}=0$, where $\vec{k}$ is the wave vector of current carriers. In this case, the effective Hamiltonian can be represented as

$$H = H_0 + \frac{\hbar}{4m_0^2c^2}[\vec{\nabla}V \times \vec{p}] \cdot \vec{\sigma} \quad (1)$$

and the corresponding (1) Schrödinger equation has the form

$$\{H_0 + \frac{\hbar}{4m_0^2c^2}[\vec{\nabla}V \times \vec{p}] \cdot \vec{\sigma}\}\psi_{n\vec{k}}(\vec{r}) = E_n(\vec{k})\psi_{n\vec{k}}(\vec{r}) \ , \quad (2)$$

where $H_0 = \frac{p^2}{2m_0} + V(r)$ consists of kinetic and potential energy operators, the second term in (1) is the spin-orbit interaction operator, $\vec{\sigma}$ is the vector of Pauli spin matrices with components:

$$\sigma_x = \begin{Bmatrix} 0 & 1 \\ 1 & 0 \end{Bmatrix} \ \sigma_y = \begin{Bmatrix} 0 - i \\ 0 \ i \end{Bmatrix} \ \sigma_z = \begin{Bmatrix} 1 & 0 \\ 0 & -1 \end{Bmatrix} \quad (3)$$

whence for the spinors $\uparrow \equiv \begin{Bmatrix} 1 \\ 0 \end{Bmatrix}$ $\downarrow \equiv \begin{Bmatrix} 0 \\ 1 \end{Bmatrix}$ we have the following relations

$$\sigma_x \uparrow = \downarrow \ \ \sigma_y \uparrow = i \downarrow \ \ \sigma_z \uparrow = \uparrow \qquad \sigma_x \downarrow = \uparrow \ \ \sigma_y \downarrow = -i \uparrow \ \ \sigma_z \downarrow = -\downarrow \quad (4)$$

If the solution (3) is sought in the form of the Bloch function $\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}}u_{n\vec{k}}(\vec{r})$,, then we obtain the equation for the Bloch amplitude $u_{n\vec{k}}(r)$ as

$$\{H_0 + \frac{\hbar}{m_0}\vec{k}\vec{p} + \frac{\hbar}{4m_0^2c^2}[\vec{\nabla}V \times \vec{p}] \cdot \vec{\sigma} + \frac{\hbar^2}{4m_0^2c^2}[\vec{\nabla}V \times \vec{k}] \cdot \vec{\sigma}\}u_{n\vec{k}}(\vec{r}) = E' u_{n\vec{k}}(r) \quad (5)$$

where $E' = E_n(\vec{k}) - \frac{\hbar^2k^2}{2m_0}$. The last term in (5) describes the spin-orbit interaction, which depends on the wave vector of current carriers. Thus, the effective Hamiltonian acting on the periodic function $u_{n\vec{k}}(r)$ is expressed as:

$$H = H_0 + \frac{\hbar}{m_0}\vec{k}\vec{p} + \frac{\hbar^2}{4m_0^2c^2}[\vec{\nabla}V \times \vec{k}] \cdot \vec{\sigma} + \frac{\hbar}{4m_0^2c^2}[\vec{\nabla}V \times \vec{p}] \cdot \vec{\sigma} \quad (6)$$

Here $H_1 = \frac{\hbar}{m_0}\vec{k}\vec{p}$ and $H_2 = \frac{\hbar^2}{4m_0^2c^2}[\vec{\nabla}V \times \vec{k}] \cdot \vec{\sigma}$ appear due to the transition from the Bloch function to the function $u_{n\vec{k}}(r)$, the term $H_3 = \frac{\hbar}{4m_0^2c^2}[\vec{\nabla}V \times \vec{p}] \cdot \vec{\sigma}$ describes $\vec{p}$ dependent in-orbit interaction. The Bloch amplitude $u_{n\vec{k}}(r)$ for electrons in the conduction band can be represented as: $|iS\uparrow\rangle$, $|iS\downarrow\rangle$, and for holes in the valence band -$|X\uparrow\rangle$, $|X\downarrow\rangle$, $|Y\uparrow\rangle$, $|Y\downarrow\rangle$, $|Z\uparrow\rangle$, $|Z\downarrow\rangle$ with the corresponding intrinsic energies E_s and E_p, which are defined as $H_0|S\rangle = E_c|S\rangle$, $H_0|X\rangle = E_p|X\rangle$, $H_0|Y\rangle = E_p|Y\rangle$, $H_0|Z\rangle = E_p|Z\rangle$, where [8]

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$$|S\rangle = \frac{1}{\sqrt{4\pi}} \quad, \ |Z\rangle = \sqrt{\frac{3}{4\pi}}\frac{z}{r}\ ,\ |X \pm iY\rangle = \sqrt{\frac{3}{4\pi}}\frac{x \pm iy}{r}, \qquad (7)$$

where it was considered that the wave function of the electrons in the conduction band is the wave function of the s-state, and for the valence band, the p-state of the hydrogen atom. Since the states in the conduction band are twofold degenerate along the spin, and in the valence band fourfold degenerate, therefore, the basic functions can be represented as:

$$|1\rangle = |iS\downarrow\rangle, |2\rangle = |\frac{X-iY}{\sqrt{2}}\uparrow\rangle, |3\rangle = |Z\downarrow\rangle, |4\rangle = |-\frac{X+iY}{\sqrt{2}}\uparrow\rangle\ , \qquad (8)$$

$$|\overline{1}\rangle = |iS\uparrow\rangle, |\overline{2}\rangle = |-\frac{X+iY}{\sqrt{2}}\downarrow\rangle, = |Z\uparrow\rangle, = |\frac{X-iY}{\sqrt{2}}\downarrow\rangle\ . \qquad (9)$$

RESULTS AND CONCLUSIONS

First, we determine the diagonal matrix elements of the Hamiltonian (6) from the basis functions (8) and (9). This requires calculating the matrix elements of each term (6) separately, where in further calculations we take into account that $\iiint_{-\infty}^{\infty}\frac{x^{2m+1}\cdot y^{l}\cdot z^{\mu}}{r^n}d\vec{r} = \iiint_{-\infty}^{\infty}\frac{x^{m}\cdot y^{2l+1}\cdot z^{\mu}}{r^n}d\vec{r} = \iiint_{-\infty}^{\infty}\frac{x^{m}\cdot y^{l}\cdot z^{2\mu+1}}{r^n}d\vec{r} = 0$, where $d\vec{r} = dxdydz$, m, l, μ are integers. Then the matrix elements of the operators

$$H_1 = \frac{\hbar}{m_0}\vec{k}\vec{p},\ H_2 = \frac{\hbar^2}{4m_0^2c^2}\left[\vec{\nabla}V \times \vec{k}\right]\cdot\vec{\sigma},\ H_3 = \frac{\hbar}{4m_0^2c^2}\left[\vec{\nabla}V \times \vec{p}\right]\cdot\vec{\sigma} \qquad (10)$$

are defined with the following relations

$$(H_0)_{11} = \langle 1|H_0|1\rangle = \langle -iS\downarrow|H_0|iS\downarrow\rangle = \langle S|E_s|S\rangle = E_s, \qquad (11)$$

$$(H_1)_{11} = \langle 1|H_1|1\rangle = \langle -iS\downarrow|H_1|iS\downarrow\rangle = \langle S|\frac{\hbar}{m_0}\vec{k}\vec{p}|S\rangle = 0, \qquad (12)$$

$$(H_2)_{11} = \langle 1|H_2|1\rangle = \langle -iS\downarrow|H_2|iS\downarrow\rangle =$$

$$= \langle -iS\downarrow|\frac{\hbar^2}{4m_0^2c^2}\left[\vec{\nabla}V \times \vec{k}\right]\cdot\vec{\sigma}|iS\downarrow\rangle = -\frac{\hbar^2}{16\pi m_0^2c^2}\mathcal{J}_1 \qquad (13)$$

where

$$\mathcal{J}_1 = \iiint_{-\infty}^{\infty}\left\{\frac{\partial V}{\partial x}k_y - \frac{\partial V}{\partial y}k_x\right\}dxdydz \qquad (14)$$

and take into account that $\vec{p}|S\rangle = 0$ (since the function S is a constant value), as well as the conditions of orthonormal spinors

$$\sigma_x\uparrow=\downarrow, \sigma_y\uparrow= i\downarrow, \sigma_z\uparrow=\uparrow,\ \sigma_x\downarrow=\uparrow, \sigma_y\downarrow= -i\uparrow,\ \sigma_z\downarrow= -\downarrow. \qquad (15)$$

If we consider that the crystalline periodic potential consists of two: even and odd terms with respect to the coordinate inversion: $V(\vec{r}) = V_{ass}(\vec{r}) + V_{sim}(\vec{r})$, where $V_{sim}(\vec{r})V(\vec{r}) = (\overline{-}\vec{r})$, $V_{ass}(\vec{r}) = -V_{ass}(-\vec{r})$, $V_{ass}(\vec{r})$, then it is easy to verify that the integral $\mathcal{J}_1$ has nonzero terms. Therefore, we analyze the following cases.

It follows from (14) that: a) if $V(\vec{r})$ has an odd term with respect to z, then $\mathcal{J}_1 = 0$; b) if $V(\vec{r})$ has an odd term with respect to x, then $\mathcal{J}_{11} \neq 0$; c) if $V(\vec{r})$ has an odd term with respect to y, then $\mathcal{J}_{12} \neq 0$; e) if $V(\vec{r})$ has an odd term with respect to x and y, then $\mathcal{J}_1 \neq 0$.

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$$(H_3)_{11} = \langle -iS\downarrow|H_3|iS\downarrow\rangle = \langle -iS\downarrow|\frac{\hbar}{4m_0^2c^2}[\vec{\nabla}V\times\vec{p}]\cdot\vec{\sigma}|iS\downarrow\rangle =$$

$$= -\frac{\hbar}{4m_0^2c^2}\langle S\left|\left[\vec{\nabla}V\times\vec{p}\right]_z\right|S\rangle = 0 \quad (16)$$

The diagonal matrix elements of the effective Hamiltonian are defined by the following expressions:

$$(H_0)_{22} = \{\frac{X+iY}{\sqrt{2}}|H_0|\frac{X-iY}{\sqrt{2}}\} = E_p \ , \quad (17)$$

$$(H_1)_{22} = \langle\frac{X+iY}{\sqrt{2}}\uparrow|H_1|\frac{X-iY}{\sqrt{2}}\uparrow\rangle = \mathcal{J}_{22}^{(1)} + \mathcal{J}_{22}^{(2)} + \mathcal{J}_{22}^{(3)} + \mathcal{J}_{22}^{(4)}.$$

where

$$\mathcal{J}_{22}^{(1)} = -\frac{\hbar^2}{4m_0^2c^2}\frac{1}{i}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{x^2yk_y + (xy^2+xz^2)k_X\right\}dxdydz,$$

$$\mathcal{J}_{22}^{(2)} = +\frac{\hbar^2}{4m_0^2c^2}\frac{1}{i}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{(yx^2+yz^2)k_y + xy^2k_X\right\}dxdydz,$$

$$\mathcal{J}_{22}^{(3)} = -\frac{\hbar^2}{4m_0^2c^2}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{(x^3+xz^2)k_y + x^2yk_X\right\}dxdydz,$$

$$\mathcal{J}_{22}^{(4)} = -\frac{\hbar^2}{4m_0^2c^2}\frac{1}{i}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{xy^2k_y + (y^3+yz^2)k_X\right\}dxdydz,$$

whence it is clear that: a) $\mathcal{J}_{22}^{(1)}$ consists of three terms, the first of which is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$, and the second is different from zero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$; b) $\mathcal{J}_{22}^{(2)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$; c) $\mathcal{J}_{22}^{(3)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{sim}(z)$; d) $\mathcal{J}_{22}^{(4)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$.

$$(H_2)_{22} = \langle\frac{X+iY}{\sqrt{2}}\uparrow|H_2|\frac{X-iY}{\sqrt{2}}\uparrow\rangle == \mathcal{R}_{22}^{(1)} + \mathcal{R}_{22}^{(2)} + \mathcal{R}_{22}^{(3)} + \mathcal{R}_{22}^{(4)}, \quad (18)$$

where

$$\mathcal{R}_{22}^{(1)} = \frac{\hbar^2}{4m_0^2c^2}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^2}\left\{x^2\frac{\partial V}{\partial x}k_y - x^2\frac{\partial V}{\partial y}k_x\right\}dxdydz,$$

$$\mathcal{R}_{22}^{(2)} = \frac{(-i)\hbar^2}{4m_0^2c^2}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^2}\left\{xy\frac{\partial V}{\partial x}k_y - xy\frac{\partial V}{\partial y}k_x\right\}dxdydz,$$

$$\mathcal{R}_{22}^{(3)} = \frac{i\hbar^2}{4m_0^2c^2}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^2}\left\{xy\frac{\partial V}{\partial x}k_y - xy\frac{\partial V}{\partial y}k_x\right\}dxdydz,$$

$$\mathcal{R}_{22}^{(4)} = \frac{\hbar^2}{4m_0^2c^2}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^2}\left\{y^2\frac{\partial V}{\partial x}k_y - y^2\frac{\partial V}{\partial y}k_x\right\}dxdydz.$$

The last relations show that: a) $\mathcal{R}_{22}^{(1)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{asim}(z)$, and the third for

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$V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$; b) $\mathcal{R}_{22}^{(2)}$ consists of three terms, the first of which is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{asim}(z)$, and the third with $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{sim}(z)$; c) $\mathcal{R}_{22}^{(3)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$, and the second and third terms are nonzero when $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{sim}(z)$; d) $\mathcal{R}_{22}^{(4)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$.

$$(H_3)_{22} = \frac{\hbar}{4m_0^2c^2}\{\mathfrak{J}_{33}^{(1)} + \mathfrak{J}_{33}^{(2)} + \mathfrak{J}_{33}^{(3)} + \mathfrak{J}_{33}^{(4)}\}$$

$$\mathfrak{J}_{33}^{(1)} = i\frac{3\hbar}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{\frac{\partial V(\vec{r})}{\partial y}zx^2 - \frac{\partial V(\vec{r})}{\partial z}x^2y\right\}dxdydz,$$

$$\mathfrak{J}_{33}^{(2)} = i\frac{3\hbar}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{\frac{\partial V(\vec{r})}{\partial y}y^2z + (yx^2 + yz^2)\frac{\partial V(\vec{r})}{\partial z}\right\}dxdydz,$$

$$\mathfrak{J}_{33}^{(3)} = +\frac{3\hbar}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{xyz\frac{\partial V(\vec{r})}{\partial y} + (x^3 + xz^2)\frac{\partial V(\vec{r})}{\partial z}\right\}dxdydz,$$

$$\mathfrak{J}_{33}^{(4)} = -\frac{3\hbar}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{xyz\frac{\partial V(\vec{r})}{\partial y} - xy^2\frac{\partial V(\vec{r})}{\partial z}\right\}dxdydz,$$

Analyzing the last relations, we have that: a) $\mathfrak{J}_{33}^{(1)}$ is nonzero at $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{asim}(z)$; b) $\mathfrak{J}_{33}^{(2)}$ consists of three terms, the first of which is nonzero at $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{asim}(z)$, and the second is nonzero at $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{asim}(z)$, and the third with $V(\vec{r}) = V_{\phi sim}(x) + V_{sim}(y) + V_{sim}(z)$; c) $\mathcal{J}_{33}^{(3)}$ consists of three terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{asim}(z)$, and the second and third terms are nonzero when $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{asim}(z)$; d) $\mathfrak{J}_{33}^{(4)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{asim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$.

Below are expressions for the matrix element of each member of the Hamiltonian. In particular, $(H_0)_{33} = \langle Z\downarrow|H_0|Z\downarrow\rangle = \langle Z|E_p|Z\rangle = E_p$ and does not depend on the parity of the crystal potential relative to the coordinates;

$$(H_1)_{33} = \langle Z\downarrow|H_1|Z\downarrow\rangle = \langle Z\downarrow\left|\frac{\hbar}{m_0}\vec{k}\vec{p}\right|Z\downarrow\rangle = <\downarrow\downarrow>\langle Z\left|\frac{\hbar}{m_0}\vec{k}\vec{p}\right|Z\rangle =$$

$$= i\frac{\hbar^2}{4m_0^2c^2}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^2}\left\{k_x(-xz^2) + k_y(-yz^2) + k_z z\frac{y^2 + x^2}{r^3}\right\}dxdydz,$$

whence we have that the first term of the last integral is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$, and the second for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$, the third is when $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{asim}(z)$.

$$(H_2)_{33} = \langle Z\downarrow|H_1|Z\downarrow\rangle = \langle Z\downarrow\left|\frac{\hbar}{m_0}\vec{k}\vec{p}\right|Z\downarrow\rangle = <\downarrow\downarrow>\langle Z\left|\frac{\hbar}{m_0}\vec{k}\vec{p}\right|Z\rangle =$$

$$= i\frac{\hbar^2}{4m_0^2c^2}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^2}\left\{k_x(-xz^2) + k_y(-yz^2) + k_z z\frac{y^2 + x^2}{r^3}\right\}dxdydz.$$

It can be seen from the last relations that the first term of the matrix element $(H_2)_{33}$ is nonzero for

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$V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$, and the second for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$, the third is when $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{asim}(z)$.

$$(H_3)_{33} = \langle Z\downarrow|H_3|Z\downarrow\rangle = \langle Z\downarrow|\frac{\hbar^2}{4m_0^2c^2}\left[\vec{\nabla}V \times \vec{p}\right]\cdot\vec{\sigma}|Z\downarrow\rangle =$$

$= -\frac{i\hbar^2}{4m_0^2c^2}\frac{3}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^4}\left\{z^2\frac{\partial V(\vec{r})}{\partial x}y - xz^2\frac{\partial V(\vec{r})}{\partial y}\right\}dxdyd$ and this matrix element is nonzero at $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{sim}(z)$.

The nondiagonal matrix elements $\langle 1|H_0|2\rangle$, $\langle 1|H_1|2\rangle$ is equal to zero, and the expression for the nondiagonal matrix elements $\langle 1|H_2|2\rangle$ and $\langle 1|H_3|2\rangle$ are given below

$$\langle 1|H_2|2\rangle = \langle 1|H_2|2\rangle = \langle -iS\downarrow|H_2|\frac{X-iY}{\sqrt{2}}\uparrow\rangle = \frac{\hbar^2}{4m_0^2c^2}\{\mathcal{J}_{21} - i\mathcal{J}_{22}\},$$

$$\langle 1|H_3|2\rangle = \langle 1|H_3|2\rangle = \langle -iS\downarrow|H_3|\frac{X-iY}{\sqrt{2}}\uparrow\rangle = \frac{\hbar}{4m_0^2c^2}(\mathcal{J}_{31} - i\mathcal{J}_{32}),$$

where

$$\mathcal{J}_{21} = \mathcal{J}_{21}^{(1)} - i\mathcal{J}_{21}^{(2)},\ \mathcal{J}_{21}^{(1)} = k_z\sqrt{\frac{1}{4\pi}}\sqrt{\frac{3}{4\pi}}\iiint_{-\infty}^{\infty}\frac{\partial V(\vec{r})}{\partial y}\frac{x-iy}{r}dxdydz,$$

$$\mathcal{J}_{21}^{(2)} = k_y\sqrt{\frac{3}{4\pi}}\sqrt{\frac{1}{4\pi}}\iiint_{-\infty}^{\infty}\frac{\partial V(\vec{r})}{\partial z}\frac{x-iy}{r}dxdydz;$$

$$\mathcal{J}_{22} = \mathcal{J}_{22}^{(1)} - i\mathcal{J}_{22}^{(2)},\ \mathcal{J}_{22}^{(1)} = k_x\sqrt{\frac{1}{4\pi}\sqrt{\frac{3}{4\pi}}}\iiint_{-\infty}^{\infty}\frac{\partial V(\vec{r})}{\partial z}\frac{x-iy}{r}dxdydz,$$

$$\mathcal{J}_{22}^{(2)} = k_z\sqrt{\frac{3}{4\pi}}\sqrt{\frac{1}{4\pi}}\iiint_{-\infty}^{\infty}\frac{\partial V(\vec{r})}{\partial x}\frac{x-iy}{r}\frac{x-iy}{r}dxdydz;$$

$$\mathcal{J}_{31} = \langle S\left|\left[\vec{\nabla}V \times \vec{p}\right]_x\right|\frac{X-iY}{\sqrt{2}}\rangle = \mathcal{J}_{32}^{(1)} - \mathcal{J}_{31}^{(2)},$$

$$\mathcal{J}_{31}^{(1)} = \frac{\hbar}{i}\sqrt{\frac{1}{4\pi}}\sqrt{\frac{3}{4\pi}}\iiint_{-\infty}^{\infty}\left\{\frac{\partial V(\vec{r})}{\partial y}\right\}(-1)\frac{z}{r}\frac{x-iy}{r^2}dxdydz,$$

$$\mathcal{J}_{31}^{(2)} = \frac{\hbar}{i}\sqrt{\frac{1}{4\pi}}\sqrt{\frac{3}{4\pi}}\iiint_{-\infty}^{\infty}\left\{\frac{\partial V(\vec{r})}{\partial z}\right\}\frac{1}{r^3}\{-i(x^2+z^2) - yx\}\,dxdydz;$$

$$\mathcal{J}_{32} = \langle S\left|\left[\vec{\nabla}V \times \vec{p}\right]_y\right|\frac{X-iY}{\sqrt{2}}\rangle = \mathcal{J}_{32}^{(1)} - \mathcal{J}_{32}^{(2)},$$

$$\mathcal{J}_{32}^{(1)} = \frac{\hbar}{i}\sqrt{\frac{1}{4\pi}}\sqrt{\frac{3}{2\pi}}\iiint_{-\infty}^{\infty}\left\{\frac{\partial V(\vec{r})}{\partial z}\right\}\frac{1}{r^3}\{y^2+z^2 - iyx\}\,dxdydz,$$

$$\mathcal{J}_{32}^{(2)} = \frac{\hbar}{i}\sqrt{\frac{1}{4\pi}}\sqrt{\frac{3}{4\pi}}\iiint_{-\infty}^{\infty}\left\{\frac{\partial V(\vec{r})}{\partial x}\right\}(-1)\frac{z}{r}\frac{x-iy}{r^2}dxdydz,$$

whence it is clear that the nonzero values of these matrix elements are determined by the physical nature, i.e. depending on the coordinate of the crystalline potential: $V(\vec{r}) = V_{ass}(\vec{r}) + V_{sim}(\vec{r})$.

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Now we analyze the functions of $\mathcal{J}_{lm}$: a) $\mathcal{J}_{21}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{sim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{asim}(z)$; b) $\mathcal{J}_{22}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{asim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$; c) $\mathcal{J}_{21}^{(1)}$ differs from zero for $V(\vec{r}) = V_{asim}(x,) + V_{sim}(y) + V_{sim}(z)$; d) $\mathcal{J}_{21}^{(2)}$ and $\mathcal{J}_{22}^{(1)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{asim}(z)$, and the second is not equal to zero when $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{asim}(z)$; e) $\mathcal{J}_{22}^{(2)}$ consists of two terms, the first of which is is not equal to zero when $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{sim}(z)$, and the second is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{sim}(z)$; f) $\mathcal{J}_{31}^{(1)}$ consists of two terms, the first of which is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{asim}(z)$, and the second is differs from zero at $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{asim}(z)$; g) $\mathcal{J}_{31}^{(2)}$ consists of two terms, the first of which is nonzero at $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{asim}(z)$, and the second is differs from zero at $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{asim}(z)$; i) $\mathcal{J}_{32}^{(1)}$ consists of two terms, the first of which is not equal to zero when $V(\vec{r}) = V_{sim}(x) + V_{sim}(y) + V_{asim}(z)$, and the second is nonzero at $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{asim}(z)$; k) $\mathcal{J}_{32}^{(2)}$ consists of two terms, the first of which is differs from zero at $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{asim}(z)$, and the second is not equal to zero when $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{asim}(z)$.

Similarly, we obtain the expressions for the following matrix elements: $(H_0)_{13} = \langle 1|H|3\rangle = \langle -iS\downarrow|H|Z\downarrow\rangle = 0$, $(H_1)_{13} = \langle -iS\downarrow|H_1|Z\downarrow\rangle = -i\langle S|\frac{\hbar}{m_0}\vec{k}\vec{p}|Z\rangle = k_z\wp_z$, where $\wp_z = -\frac{\hbar^2}{m_0}\frac{\sqrt{3}}{4\pi}\iiint_{-\infty}^{\infty}\frac{x^2+y^2}{r^3}dxdydz$. А также

and

$$(H_2)_{13} = \langle -iS\downarrow|H_2|Z\downarrow\rangle = \langle -iS\downarrow|\frac{\hbar^2}{4m_0^2c^2}\left[\vec{\nabla}V\times\vec{k}\right]\cdot\vec{\sigma}|Z\downarrow\rangle =$$

$$= i\frac{\hbar^2}{4m_0^2c^2}\frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{4\pi}}\iiint_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}k_y - \frac{\partial V}{\partial y}k_x\right)\frac{z}{r}dxdydz,$$

It can be seen from the latter that the first term is nonzero for $V(\vec{r}) = V_{asim}(x) + V_{sim}(y) + V_{asim}(z)$, and the second term is nonzero for $V(\vec{r}) = V_{sim}(x) + V_{asim}(y) + V_{asim}(z)$. Also

$$(H_3)_{13} = \langle -iS\downarrow|H_3|Z\downarrow\rangle = -(-i)\frac{\hbar}{4m_0^2c^2}\langle S\left|\left[\vec{\nabla}V\times\vec{p}\right]_z\right|Z\rangle =$$

$$= -\frac{\hbar^2}{4m_0^2c^2}\frac{\sqrt{3}}{4\pi}\iiint_{-\infty}^{\infty}\frac{1}{r^3}\left\{yz\frac{\partial V}{\partial x} - xz\frac{\partial V}{\partial y}\right\}dxdydz$$

whence it is clear that this matrix element is nonzero at $V(\vec{r}) = V_{asim}(x) + V_{asim}(y) + V_{asim}(z)$.

Thus, it was shown that, when the asymmetric part of the crystalline potential in semiconductors is taken into account, additional terms are obtained in the matrix elements of the effective Hamiltonian.

If we assume that the crystalline potential does not have an asymmetric part, then all the expressions obtained above and related to $V_{asim}(x,y,z)$ turn to zero automatically.

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