# A tight–binding model for $p$ electrons with spin–orbit interaction

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In the following paper we will consider a tight–binding model for $p$ zone with spin–orbit interaction.

Before we start, let us remind the Clebsch–Gordan coefficients for the case $l = 1$, $s = \frac{1}{2}$. Let $a_{j,m}$ annihilate the state with angular momentum $j$ and the projection $m$ ($j \in \{3/2, 1/2\}$), and $b_{m,s}$ — the state with orbital momentum projection $m$ ($j = 1$) and spin projection $s$.

$$\begin{aligned}
a_{\frac{3}{2},\frac{3}{2}} &= b_{1,\frac{1}{2}} \\
a_{\frac{3}{2},\frac{1}{2}} &= \sqrt{\frac{1}{3}} b_{1,-\frac{1}{2}} + \sqrt{\frac{2}{3}} b_{0,\frac{1}{2}} \\
a_{\frac{3}{2},-\frac{1}{2}} &= \sqrt{\frac{2}{3}} b_{0,-\frac{1}{2}} + \sqrt{\frac{1}{3}} b_{-1,\frac{1}{2}} \\
a_{\frac{3}{2},-\frac{3}{2}} &= b_{-1,-\frac{1}{2}} \\
a_{\frac{1}{2},\frac{1}{2}} &= \sqrt{\frac{2}{3}} b_{1,-\frac{1}{2}} - \sqrt{\frac{1}{3}} b_{0,\frac{1}{2}} \\
a_{\frac{1}{2},-\frac{1}{2}} &= -\sqrt{\frac{1}{3}} b_{0,-\frac{1}{2}} + \sqrt{\frac{2}{3}} b_{-1,\frac{1}{2}}
\end{aligned} \tag{1}$$

After expressing the $b$ operators using $p_x$, $p_y$ and $p_z$, we immediately obtain

$$\begin{aligned}
a_{\frac{3}{2},\frac{3}{2}} &= \sqrt{\frac{1}{2}} \left( p_{x,\frac{1}{2}} - i p_{y,\frac{1}{2}} \right) \\
a_{\frac{3}{2},\frac{1}{2}} &= \sqrt{\frac{1}{6}} \left( p_{x,-\frac{1}{2}} - i p_{y,-\frac{1}{2}} \right) + \sqrt{\frac{2}{3}} p_{z,\frac{1}{2}} \\
a_{\frac{3}{2},-\frac{1}{2}} &= \sqrt{\frac{2}{3}} p_{z,-\frac{1}{2}} + \sqrt{\frac{1}{6}} \left( p_{x,\frac{1}{2}} + i p_{y,\frac{1}{2}} \right) \\
a_{\frac{3}{2},-\frac{3}{2}} &= \sqrt{\frac{1}{2}} \left( p_{x,-\frac{1}{2}} + i p_{y,-\frac{1}{2}} \right)
\end{aligned} \tag{2}$$

$$
\begin{aligned}
a_{\frac{1}{2},\frac{1}{2}} &= \sqrt{\frac{1}{3}}\left(p_{x,-\frac{1}{2}} - ip_{y,-\frac{1}{2}}\right) - \sqrt{\frac{1}{3}}p_{z,\frac{1}{2}} \\
a_{\frac{1}{2},-\frac{1}{2}} &= -\sqrt{\frac{1}{3}}p_{z,-\frac{1}{2}} + \sqrt{\frac{1}{3}}\left(p_{x,\frac{1}{2}} + ip_{y,\frac{1}{2}}\right)
\end{aligned} \tag{3}
$$

As (2), (3) define a unitary transformation, $p$ can be easily expressed via $a$.

The Hamiltonian is

$$
\begin{aligned}
H_{\text{full}} = -\Delta E_{SO} a^{\dagger}_{\frac{1}{2},-\frac{1}{2}} a_{\frac{1}{2},-\frac{1}{2}} + \\
+ 2(t_{\parallel}\cos p_x + t_{\perp}\cos p_y) p^{\dagger}_{x,\frac{1}{2}} p_{x,\frac{1}{2}} + \\
+ 2(t_{\perp}\cos p_x + t_{\parallel}\cos p_y) p^{\dagger}_{y,\frac{1}{2}} p_{y,\frac{1}{2}} + \\
+ 2t_3(\cos p_x + \cos p_y) p^{\dagger}_{z,-\frac{1}{2}} p_{z,-\frac{1}{2}}
\end{aligned} \tag{4}
$$

It contains the atomic spin–orbit part and the part which depends on the interaction between neighbour atoms.

After simple calculation we obtain the Hamiltonian matrix in the basis of $p$ operators:

$$
\begin{aligned}
H = -\frac{E_{SO}}{3}\begin{pmatrix} 1 & i & -1 \\ -i & 1 & i \\ -1 & -i & 1 \end{pmatrix} + \\
+ \begin{pmatrix} t_{\parallel}\cos p_x + t_{\perp}\cos p_y & 0 & 0 \\ 0 & t_{\perp}\cos p_x + t_{\parallel}\cos p_y & 0 \\ 0 & 0 & t_3(\cos p_x + \cos p_y) \end{pmatrix}
\end{aligned} \tag{5}
$$

The energy levels for the case $\Delta E_{SO} = 1$, $t_{\parallel} = 0.3$, $t_3 = t_{\perp} = 0.15$ are shown on the figure.

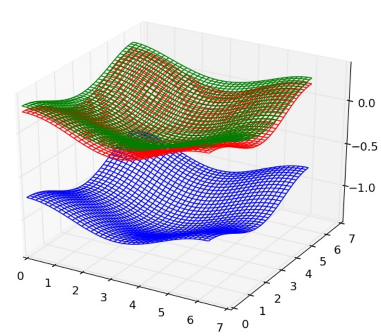


Figure 1: Energy levels

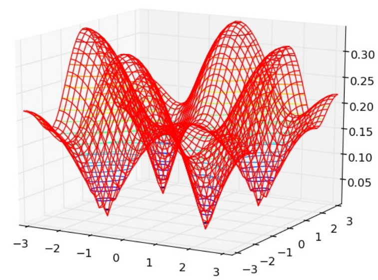


Figure 2: The difference of two upper energy levels

In some cases it would be (maybe) more convenient to write the Hamiltonian in the basis of $a$ operators. For solving that problem, the following observation would be useful.

Let $|A\rangle$ and $|B\rangle$ be the spinless states with angular momentum projections $m$ and $m'$. Let $|A\rangle$ also be localised in $(0,0)$, and $|B(\phi)\rangle$ — in $(r\cos\phi, r\sin\phi$. Then the following equation holds:

$$\langle A|B(\phi)\rangle = e^{-i(m-m')\phi}\langle A|B(0)\rangle \tag{6}$$

That allows to write any tight–binding Hamiltonian directly in terms of $a$ states.

First Let the angle be zero, and let the hopping integrals for the $b$ operators be described by matrix

$$T_b = \begin{pmatrix} t_1 & 0 & t_2 \\ 0 & t_3 & 0 \\ t_2 & 0 & t_1 \end{pmatrix} \tag{7}$$

The $t_i$ can be expressed via $t_\perp, t_\parallel$.

$$\begin{aligned} t_1 &= \frac{1}{2}\left(t_\parallel + t_\perp\right) \\ t_2 &= \frac{1}{2}\left(t_\parallel - t_\perp\right) \end{aligned} \tag{8}$$

Then for the states described by full momentum ($a$ states) we obtain

$$T_x = \begin{pmatrix} t_1 & \frac{1}{\sqrt{3}}t_2 & \sqrt{\frac{2}{3}}t_2 \\ \frac{1}{\sqrt{3}}t_2 & \frac{1}{3}(t_1+2t_3) & \frac{\sqrt{2}}{3}(t_1-t_3) \\ \sqrt{\frac{2}{3}}t_2 & \frac{\sqrt{2}}{3}(t_1-t_3) & \frac{1}{3}(2t_1+t_3) \end{pmatrix} \tag{9}$$

For the arbitrary angle, as follows from 6,

$$T_\phi = \mathrm{diag}(e^{\frac{-3i\phi}{2}}, e^{\frac{i\phi}{2}}, e^{\frac{i\phi}{2}}) \times T_x \times \mathrm{diag}(e^{\frac{3i\phi}{2}}, e^{\frac{-i\phi}{2}}, e^{\frac{-i\phi}{2}}) = \\ = \begin{pmatrix} t_1 & \frac{1}{\sqrt{3}} t_2 e^{-2i\phi} & \sqrt{\frac{2}{3}} t_2 e^{-2i\phi} \\ \frac{1}{\sqrt{3}} t_2 e^{2i\phi} & \frac{1}{3}(t_1 + 2t_3) & \frac{\sqrt{2}}{3}(t_1 - t_3) \\ \sqrt{\frac{2}{3}} t_2 e^{2i\phi} & \frac{\sqrt{2}}{3}(t_1 - t_3) & \frac{1}{3}(2t_1 + t_3) \end{pmatrix} \tag{10}$$

The Hamiltonian is now

$$H = \mathrm{diag}\,(0, 0, -\Delta E_{SO}) + 2\cos p_x T_0 + 2\cos p_y T_{\frac{\pi}{2}} + \\ + 2\cos(p_x + p_y)\tilde{T}_{\frac{\pi}{4}} + 2\cos(p_x - p_y)\tilde{T}_{-\frac{\pi}{4}} + \dots \tag{11}$$

We will treat the first term as the unperturbed system and all other as a perturbation. The unperturbed Hamiltonian has a pair of degenerate levels. The non–trivial topology can only exist due to "entaglement" of these levels. As we treat the $T$ matrices as a perturbation, we will find the eigenfunctions and eigenvalues of the restricted perturbation matrix $V$.

$$V = 2 \begin{pmatrix} t_1(\cos p_x + \cos p_y) + 2\tilde{t}_1 \cos p_x \cos p_y & \frac{1}{\sqrt{3}} t_2(\cos p_x - \cos p_y) + \frac{2i}{\sqrt{3}} \tilde{t}_2 \sin p_x \sin p_y \\ \frac{1}{\sqrt{3}} t_2(\cos p_x - \cos p_y) + \frac{2i}{\sqrt{3}} \tilde{t}_2 \sin p_x \sin p_y & \frac{1}{3}(t_1 + 2t_3)(\cos_{p_x} + \cos p_y) + \frac{2}{3}(\tilde{t}_1 + 2\tilde{t}_3)\cos_{p_x}\cos_{p_y} \end{pmatrix} = \\ = \begin{pmatrix} a & b \\ b* & c \end{pmatrix} \tag{12}$$