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.

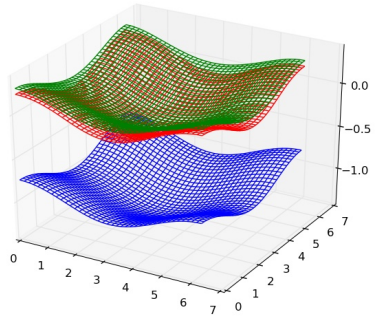

Figure 1: Energy levels

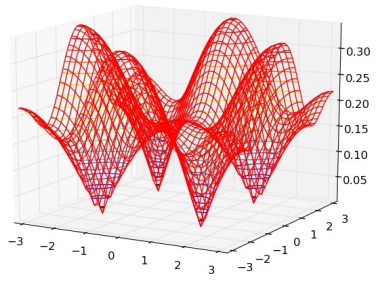

Figure 2: The difference of two upper energy levels

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,

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

The Hamiltonian is now

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

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.

$$V = \begin{pmatrix} a & b \\ b^* & c \end{pmatrix}, \quad \text{where} \\ \begin{aligned} a &= 2t_1(\cos p_x + \cos p_y) + 4\tilde{t}_1 \cos p_x \cos p_y, \\ b &= \frac{2t_2}{\sqrt{3}}(\cos p_x - \cos p_y) + \frac{4i\tilde{t}_2}{\sqrt{3}} \sin p_x \sin p_y \\ c &= \frac{2}{3}(t_1 + 2t_3)(\cos p_x + \cos p_y) + \frac{4}{3}(\tilde{t}_1 + 2\tilde{t}_3)\cos p_x \cos p_y \end{aligned} \quad (12)$$

The eigenvalues are

$$\epsilon = \frac{a + c \pm \sqrt{(a-c)^2 + 4|b|^2}}{2} \quad (13)$$

As can be seen from the structure of a, b, c coefficients, the gap between the bands doesn't vanish unless $a = c$ and $b = 0$ simultaneously. This is quite a special case and we will not consider it. Let us select, for example, the upper band. We can write two expressions for an eigenvector corresponding to p_x, p_y:

$$\begin{aligned} v_1 &= \frac{1}{\sqrt{(\epsilon - a)^2 + |b|^2}} \begin{pmatrix} b \\ \epsilon - a \end{pmatrix} \\ v_2 &= \frac{1}{\sqrt{(\epsilon - c)^2 + |b|^2}} \begin{pmatrix} \epsilon - c \\ b^* \end{pmatrix} \end{aligned} \quad (14)$$

The only difference between v_1, v_2 is in the phase multiplier $e^{i\phi}$:

$$e^{i\phi} = \frac{\epsilon - c}{b} \sqrt{\frac{(\epsilon - a)^2 + |b|^2}{(\epsilon - c)^2 + |b|^2}} = \frac{b^*}{\epsilon - a} \sqrt{\frac{(\epsilon - a)^2 + |b|^2}{(\epsilon - c)^2 + |b|^2}} \quad (15)$$

The multiplier is well–defined when $b \neq 0$, and, as follows, outside the points $(p_x, p_y) = (0,0)$ or $(p_x, p_y) = (\pi, \pi)$.

So we can consider its behavoir on a closed line (a small circle, for example) wrapping around the point $(p_x, p_y) = (0,0)$. Obviously, $e^{i\phi} = e^{-i \operatorname{Arg} b}$. At small p,

$$b = \frac{t_2}{\sqrt{3}}(p_x^2 - p_y^2) + \frac{4i\tilde{t}_2}{3} p_x p_y + o(p^2) \tag{16}$$

After substituting $p_x = p\cos\alpha$, $p_y = p\sin\alpha$ we obtain

$$b = \frac{t_2 p^2}{\sqrt{3}} \cos 2\alpha + \frac{2i\tilde{t}_2 p^2}{3} \sin 2\alpha + o(p^2) \tag{17}$$

Now it is obvious that the phase of $e^{i\phi}$ changes by 4π after p turns around $(0,0)$. So, the Hamiltonian describes a topological insulator. However, as the index is odd, the total Hamiltonian (which includes spin up and down) is topologically trivial.

1 The Hamiltonian with p and s-type orbitals

The Hamiltonian written below is quite naive: it includes the overlapping p and s orbitals and the spin–orbit interaction.

$$\begin{aligned} H = \sum & (E_s + 4t_s) s^\dagger_{mn} s_{mn} - t_s s^\dagger_{mn}(s_{m+1,n} + s_{m-1,n} + s_{m,n+1} + s_{m,n-1}) \\ & + t_{sp} s^\dagger_{mn}(-p^x_{m+1,n} + p^x_{m-1,n} - p^y_{m,n+1} + p^y_{m,n-1}) + \text{h.c.} \\ & + (p^x_{mn})^\dagger (t_\parallel (p^x_{m+1,n} + p^x_{m-1,n}) + t_\perp (p^x_{m,n+1} + p^x_{m,n-1})) \\ & + (p^x_{mn})^\dagger (t_\perp (p^y_{m+1,n} + p^y_{m-1,n}) + t_\parallel (p^y_{m,n+1} + p^y_{m,n-1})) \\ & + (p^z_{mn})^\dagger t_3 (p^z_{m+1,n} + p^z_{m-1,n} + p^z_{m,n+1} + p^z_{m,n-1}) \\ & - \frac{E_{SO}}{3} \begin{pmatrix} p_x^\dagger & p_y^\dagger & p_z^\dagger \end{pmatrix} \begin{pmatrix} 1 & i & -1 \\ -i & 1 & i \\ -1 & -i & 1 \end{pmatrix} \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} \end{aligned} \tag{18}$$