Friday, Oct. 28-th, 2016:

Kane - derivation:

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$$

$$\hat{H} = \left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{\hbar}{m}\vec{k}\cdot\vec{p} + \frac{\hbar^2}{4mc^2}(\nabla V \times \vec{p})\cdot\hat{\vec{\sigma}} + V(\vec{r})\right]$$

Listing the Pauli - spin matrices:

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};\ \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};\ \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$(\nabla V \times \vec{p})\cdot\vec{\sigma} = \left(\sum_i \frac{\partial V}{\partial x_i}\hat{x}_i \times \sum_j p_j \hat{x}_j\right)\cdot\hat{\vec{\sigma}}$$

$$= \sum_{i,j} \frac{\partial V}{\partial x_i} p_j (\hat{x}_i \times \hat{x}_j)\cdot\hat{\vec{\sigma}}$$

$$= \hat{\sigma}_k \sum_{i,j} \epsilon_{ijk} \frac{\partial V}{\partial x_i} p_j$$

& $\vec{k}\cdot\vec{p} = \sum_i k_i p_i = k \sum_i \hat{p}_i$

We focus just on the 4×4 block H, as in Kane's paper, we diagonalize w/ Cartesian basis $|iS\downarrow\rangle$, $\frac{1}{\sqrt{2}}|X-iY\rangle$, $|Z\downarrow\rangle$, $|X+iY\rangle/\sqrt{2}$.

$$H_{11} = \langle iS\downarrow|\hat{H}|iS\downarrow\rangle$$

$\because \langle s|\hat{\vec{k}}\cdot\hat{\vec{p}}|s\rangle = 0$ & $\langle S|(\nabla V\times\vec{p})|S\rangle = 0$ because $|S\rangle$ has no position dependence,

$$H_{11} = \langle iS\downarrow|\hat{H}_0|iS\downarrow\rangle = \langle S|H_0|S\rangle\overbrace{(-i\cdot i)}^{=1}$$

$= \underline{E_g}$ ✓ (which Kane defines as the conduction band energy @ the band minimum @ $\vec{k}=0$)

$$H_{12} = \langle iS\downarrow|\hat{H}|(X-iY)/\sqrt{2}\rangle$$
$$= \frac{-i}{\sqrt{2}}\langle S\downarrow|\hat{H}|X\uparrow\rangle - \langle S\downarrow|\hat{H}|Y\uparrow\rangle/\sqrt{2}$$

Looking @ just one of these terms, $\langle S\downarrow|\hat{H}|X\uparrow\rangle$
$\propto \langle S|(\hat{\vec{k}}\cdot\hat{\vec{p}})|X\rangle\langle\downarrow|\uparrow\rangle$ ... ($\because$ no other terms couple these states)

$= \underline{0}$.

Thus, $\underline{H_{12} = 0}$ ✓

$$H_{13} = \langle iS\downarrow | \left(\frac{\hbar \vec{k}}{m}\cdot \vec{p}\right) | Z\downarrow \rangle$$

$$= -i \langle S | \vec{k}\cdot\vec{p} | Z \rangle \cdot \frac{\hbar}{m} \overbrace{\langle \downarrow | \downarrow \rangle}^{=1}$$

$$= -i\frac{\hbar k}{m} \langle S | \hat{p}_z | Z \rangle = \underline{-kP} \checkmark$$

where $P = \frac{i\hbar}{m} \langle S | \hat{p}_z | Z \rangle$

$$H_{14} = \langle iS\downarrow | \hat{H} | (X+iY)\uparrow/\sqrt{2} \rangle = \underline{0} \checkmark \quad (\text{Like } H_{12})$$

$$H_{21} = 0 \quad (\text{Like } H_{12}, H_{14})$$

$$H_{22} = \langle (X-iY)\uparrow/\sqrt{2} | \hat{H} | (X-iY)/\sqrt{2} \rangle$$

$$= \frac{1}{2}\Big[\underbrace{\langle X | \hat{H}_0 | X \rangle + \langle Y | \hat{H}_0 | Y \rangle}_{=E_p} + \langle -iY\uparrow | \hat{H} | X \rangle \ldots$$

$$\ldots + \langle X | \hat{H} | -iY \rangle \Big]$$

$$= E_p - \frac{i}{2}\left(\langle X | H | Y \rangle \cdot 2\right) \overbrace{\langle \uparrow | \hat{\sigma}_z | \uparrow \rangle}^{=1}$$

$$= E_p - i\left(\langle X | \left(\frac{\partial V}{\partial x} p_y - \frac{\partial V}{\partial y} p_x\right) | Y \rangle\right) \frac{\hbar}{4m^2c^2}$$

$$= \underline{E_p - \Delta/3} \checkmark \quad (\text{with Kane's definitions})$$

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$$H_{23} = \langle (X - iY)\uparrow/\sqrt{2} \,|\, \hat{H} \,|\, Z\downarrow \rangle$$

Now, let's look at:

$$\langle \uparrow | \hat{\sigma}_y | \downarrow \rangle = (1\ 0)\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -i$$

&,

$$\langle \uparrow | \hat{\sigma}_x | \downarrow \rangle$$

$$= (1\ 0)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \underline{1} \checkmark$$

Thus,

$$H_{23} = \frac{\hbar^2}{\sqrt{2}\,4mc^2}\Big[\langle X | \left(\frac{\partial V}{\partial z} p_x - \frac{\partial V}{\partial x} p_z\right) | Z \rangle \langle \uparrow | \hat{\sigma}_y | \downarrow \rangle \ldots$$

$$\ldots + i \langle Y | \left(\frac{\partial V}{\partial y} p_z - \frac{\partial V}{\partial z} p_y\right) | Z \rangle \langle \uparrow | \hat{\sigma}_x | \downarrow \rangle \Big]$$

$$= \frac{1}{\sqrt{2}}\left[\frac{i\hbar^2}{4mc^2} \langle Z | \left(\frac{\partial V}{\partial z} p_x - \frac{\partial V}{\partial x} p_z\right) | \cancel{X} \rangle + \frac{i\hbar^2}{4mc^2} \langle Y | \left(\frac{\partial V}{\partial y} p_z - \frac{\partial V}{\partial z} p_y\right) | Z \rangle \right]$$

$$= \frac{1}{\sqrt{2}} \cdot \frac{2\Delta}{3} = \underline{\frac{\sqrt{2}\,\Delta}{3}} \checkmark$$

Other components can be computed like-wise.