The series “Missing chapters of Juliana’s THESIS”

Tight-binding model of an isolated GaSe double layer

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In order to analyse the trends behind the band structures of “real” GeSe or InSe polytypes, consider a two-dimensional model of an isolated double layer, with only one (s-) orbital per site and nearest-neighbours interactions only. The generalization over more orbitals and / or more distant interactions is not easy but straightforward. The scheme of the layer is shown in the Figure. The notation “A” refers to cations and “B” – to anions. The anions can interact only via cations (no B-B couplings), whereas the cations participate, in addition to the A-B, in the direct A-A coupling. As a limiting case, the model can be reformulated to describe the anion-cation-anion sheet structure, i.e. MoS_2, by simply removing the A-A interactions and merging the corresponding columns/lines.

The starting point of the model is a case of isolated atoms A and B. The corresponding (non perturbed) Hamiltonian $\mathcal{H}$ yields eigenfunctions $|\alpha\rangle$ (for A) and $|\beta\rangle$ (for B) along with corresponding eigenvalues:

$$\mathcal{H}_0^{\mathrm{A}}|\alpha\rangle = \left[-\frac{\mathbf{p}^2}{2m} + V^{\mathrm{A}}\right]|\alpha\rangle = \epsilon^{\mathrm{A}}|\alpha\rangle\,; \qquad \mathcal{H}_0^{\mathrm{B}}|\beta\rangle = \left[-\frac{\mathbf{p}^2}{2m} + V^{\mathrm{B}}\right]|\beta\rangle = \epsilon^{\mathrm{B}}|\beta\rangle\,.$$

These eigenvalues will serve as a basis to expand the perturbed wave functions in crystal:

$$|\varphi_{\mathbf{k}}\rangle = \frac{1}{n}\sum_{\mu} a_{\mathbf{k}\mu}|\alpha_\mu\rangle + \frac{1}{n}\sum_{\nu} b_{\mathbf{k}\nu}|\beta_\nu\rangle\,. \tag{1}$$

These eigenfunctions are solutions of the Hamiltonian with the crystalline potential (overlapping from all sites),

$$\mathcal{H}_1 = -\frac{\mathbf{p}^2}{2m} + \sum_{\mu\,\in\,\text{sites A,B}} V^{\mu} = \mathcal{H}_0^{\mu} + \sum_{\mu'\,\in\,\text{sitesA,B}\,\neq\,\mu} V^{\mu'} \;\equiv\; \mathcal{H}_0^{\mu} + V_{\mathrm{A}}^{\mu}\,.$$

The last term is the crystal potential coming about from the summation over all crystal sites (of both species) with the exception of the potential of type A missing in site μ. Alternatively, $\mathcal{H}_1 = \mathcal{H}_0^{\nu} + V_{\mathrm{B}}^{\nu}$. Taking into account Eq. (1),

$$\mathcal{H}_1|\psi_{\mathbf{k}}\rangle = \frac{1}{n}\sum_{\mu} a_{\mathbf{k}\mu}\left[\epsilon^{\mathrm{A}} + V_{\mathrm{A}}^{\mu}\right]|\alpha_\mu\rangle + \frac{1}{n}\sum_{\nu} b_{\mathbf{k}\nu}\left[\epsilon^{\mathrm{B}} + V_{\mathrm{B}}^{\nu}\right]|\beta_\nu\rangle\,,$$

so that

$$\sum_{\mu} a_{\mathbf{k}\mu}\left[\epsilon^{\mathrm{A}} + V_{\mathrm{A}}^{\mu}\right]|\alpha_\mu\rangle + \sum_{\nu} b_{\mathbf{k}\nu}\left[\epsilon^{\mathrm{B}} + V_{\mathrm{B}}^{\nu}\right]|\beta_\nu\rangle = \epsilon_{\mathbf{k}}\left[\sum_{\mu} a_{\mathbf{k}\mu}|\alpha_\mu\rangle + \sum_{\nu} b_{\mathbf{k}\nu}|\beta_\nu\rangle\right]\,.$$

Integrating this system with $\langle\alpha_{\mu'}|$ yields:

$$\begin{aligned}\sum_{\mu} a_{\mathbf{k}\mu}\Big[\epsilon^{\mathrm{A}}\underbrace{\langle\alpha_{\mu'}|\alpha_\mu\rangle}_{S_{\mu'\mu}} + \underbrace{\langle\alpha_{\mu'}|V_{\mathrm{A}}^{\mu}|\alpha_\mu\rangle}_{T_{\mu'\mu}}\Big] + \sum_{\nu} b_{\mathbf{k}\nu}\Big[\epsilon^{\mathrm{B}}\underbrace{\langle\alpha_{\mu'}|\beta_\nu\rangle}_{S_{\mu'\nu}} + \underbrace{\langle\alpha_{\mu'}|V_{\mathrm{B}}^{\nu}|\beta_\nu\rangle}_{T_{\mu'\nu}}\Big] \\ = \epsilon_{\mathbf{k}}\Big[\sum_{\mu} a_{\mathbf{k}\mu}\underbrace{\langle\alpha_{\mu'}|\alpha_\mu\rangle}_{S_{\mu'\mu}} + \sum_{\nu} b_{\mathbf{k}\nu}\underbrace{\langle\alpha_{\mu'}|\beta_\nu\rangle}_{S_{\mu'\nu}}\Big]\,,\end{aligned} \tag{2}$$

and integrating with $\langle\beta_{\nu'}|$:

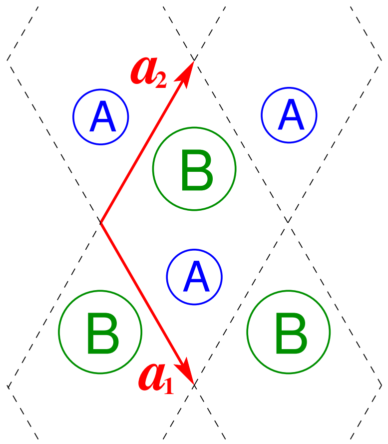
$$\sum_\mu a_{\mathbf{k}\mu}\Big[\epsilon^{\mathrm{A}}\underbrace{\langle\beta_{\nu'}|\alpha_\mu\rangle}_{S_{\nu'\mu}}+\underbrace{\langle\beta_{\nu'}|V_{\mathrm{A}}^{\mu}|\alpha_\mu\rangle}_{T_{\nu'\mu}}\Big]+\sum_\nu b_{\mathbf{k}\nu}\Big[\epsilon^{\mathrm{B}}\underbrace{\langle\beta_{\nu'}|\beta_\nu\rangle}_{\delta_{\nu'\nu}}+\underbrace{\langle\beta_{\nu'}|V_{\mathrm{B}}^{\nu}|\beta_\nu\rangle}_{T_{\nu'\nu}}\Big]$$
$$=\epsilon_{\mathbf{k}}\Big[\sum_\mu a_{\mathbf{k}\mu}\underbrace{\langle\beta_{\nu'}|\alpha_\mu\rangle}_{S_{\nu'\mu}}+\sum_\nu b_{\mathbf{k}\nu}\underbrace{\langle\beta_{\nu'}|\beta_\nu\rangle}_{\delta_{\nu'\nu}}\Big]\,. \tag{3}$$

Note that the overlap of anion-anion basis functions is non-zero only on-site, $\langle\beta_{\nu'}|\beta_\nu\rangle=\delta_{\nu'\nu}$. Equations (2) and (3) make an infinite coupled system. It can be decoupled introducing an explicite dependence on $\mathbf{k}$, i.e., the numeration of sites μ, ν will be replaced by the numeration of unit cells, and for the latter we use the Bloch periodicity condition:

$$a_{\mathbf{k}\mu}\ \Rightarrow\ a_{n,m}(\mathbf{k})=a_{0,0}(\mathbf{k})e^{i\mathbf{k}(n\mathbf{a}_1+m\mathbf{a}_2)}\,;\qquad b_{\mathbf{k}\mu}\ \Rightarrow\ b_{n,m}(\mathbf{k})=b_{0,0}(\mathbf{k})e^{i\mathbf{k}(n\mathbf{a}_1+m\mathbf{a}_2)}\,. \tag{4}$$

We specify that $a_{n,m}(\mathbf{k})$ is the coefficient with which the basis function at site A in the unit cell (n,m) enters the resulting Bloch wavefunction $|\varphi_{\mathbf{k}}\rangle$, and $b_{n,m}(\mathbf{k})$ – the same for the site B. In fact there are two A atoms and two B atoms in each unit cell which we now want to distinguish attributing the Up/Down labels to their coefficients, i.e., a^{U}_{nm} and a^{D}_{nm}, similarly for b_{nm}. This will help to construct a closed system of equations on four coefficients, bringing in the explicit dependence on $\mathbf{k}$ by force of the relations (4). When selecting non-zero interactions to be left in the system, we take into account the following rules:

– a^{U}_{nm} couples (overlaps) with itself and with its counterpart a^{D}_{nm} in the same unit cell;
– a^{U}_{nm} couples (overlaps) with three b^{U}_{nm}, one in the same cell and two in adjacent cells, similarly a^{D}_{nm} couples with three b^{D}_{nm},;
– a^{U} do not interact with b^{D};
– b's only couple to a's and not to other b's.
We assume that all basis functions are normalized, so that all on-site overlaps are 1. Nearest-neighbours overlaps S^{AA} and S^{AB}, on-site transfer integrals t^{A} and t^{B} and nearest-neighbour transfer integrals T^{AA} and T^{AB} remain the parameters of the model.



It rests to specify which sites / unit cells enter the summation over the nearest neighbours. In the placement of atoms within the unit cell as in the Figure, the A site of the reference cell (n,m) has B-type neighbours in the same cell, in the cell $(n+1,m)$ and in the cell $(n,m-1)$. In its turn, the B site of the (n,m) cell has A-neighbours in the same cell, in the cell $(n-1,m)$ and in the cell $(n,m+1)$. Therefore, the summations over ν in Eq. (2) amount to multiplying by $(1+e^{i\mathbf{k}\mathbf{a}_1}+e^{-i\mathbf{k}\mathbf{a}_2})$, and the summations over μ in Eq. (3) – to multiplying by $(1+e^{-i\mathbf{k}\mathbf{a}_1}+e^{i\mathbf{k}\mathbf{a}_2})$. The μ summation in Eq. (2) runs over this same atom A and its nearest cation neighbor, yielding the on-site overlap =1 and nearest-neighbour overlap S^{AA}, along with on-site and nearest-neighbour transfer integrals t^{A} and T^{AA}, correspondingly.

We spicify now that, in a given unit cell (n,m), there are four coefficients $a^{\mathrm{U}}_{mn}(\mathbf{k})$, $a^{\mathrm{D}}_{mn}(\mathbf{k})$, $b^{\mathrm{U}}_{mn}(\mathbf{k})$, $b^{\mathrm{D}}_{mn}(\mathbf{k})$. They are coupled such that the the equalities (2) and (3) must hold for every unit cell. This leads to four coupled equations on the coefficients (skipping the implicit $\mathbf{k}$-dependence of the latter). Eq. (2), for $\mu' = a^{\mathrm{U}}_{mn}$:

$$\begin{aligned} a^{\mathrm{U}}_{mn}(\epsilon^{\mathrm{A}}+t^{\mathrm{A}}) + a^{\mathrm{D}}_{mn}(\epsilon^{\mathrm{A}}S^{\mathrm{AA}}+T^{\mathrm{AA}}) + b^{\mathrm{U}}_{mn}(1+e^{i\mathbf{k}\mathbf{a}_1}+e^{-i\mathbf{k}\mathbf{a}_2})(\epsilon^{\mathrm{B}}S^{\mathrm{AB}}+T^{\mathrm{BA}}) \\ = \epsilon_{\mathbf{k}}\Big[a^{\mathrm{U}}_{mn} + a^{\mathrm{D}}_{mn}S^{\mathrm{AA}} + b^{\mathrm{U}}_{mn}(1+e^{i\mathbf{k}\mathbf{a}_1}+e^{-i\mathbf{k}\mathbf{a}_2})S^{\mathrm{AB}}\Big]\,; \end{aligned} \tag{5}$$

Eq. (2), for $\mu' = a^{\mathrm{D}}_{mn}$:

$$\begin{aligned} a^{\mathrm{D}}_{mn}(\epsilon^{\mathrm{A}}+t^{\mathrm{A}}) + a^{\mathrm{U}}_{mn}(\epsilon^{\mathrm{A}}S^{\mathrm{AA}}+T^{\mathrm{AA}}) + b^{\mathrm{D}}_{mn}(1+e^{i\mathbf{k}\mathbf{a}_1}+e^{-i\mathbf{k}\mathbf{a}_2})(\epsilon^{\mathrm{B}}S^{\mathrm{AB}}+T^{\mathrm{BA}}) \\ = \epsilon_{\mathbf{k}}\Big[a^{\mathrm{D}}_{mn} + a^{\mathrm{U}}_{mn}S^{\mathrm{AA}} + b^{\mathrm{D}}_{mn}(1+e^{i\mathbf{k}\mathbf{a}_1}+e^{-i\mathbf{k}\mathbf{a}_2})S^{\mathrm{AB}}\Big]\,; \end{aligned} \tag{6}$$

Eq. (3), for $\nu' = b^{\mathrm{U}}_{mn}$:

$$\begin{aligned} a^{\mathrm{U}}_{mn}(1+e^{-i\mathbf{k}\mathbf{a}_1}+e^{i\mathbf{k}\mathbf{a}_2})(\epsilon^{\mathrm{A}}S^{\mathrm{AB}}+T^{\mathrm{AB}}) + b^{\mathrm{U}}_{mn}(\epsilon^{\mathrm{B}}+t^{\mathrm{B}}) \\ = \epsilon_{\mathbf{k}}\Big[a^{\mathrm{U}}_{mn}(1+e^{-i\mathbf{k}\mathbf{a}_1}+e^{i\mathbf{k}\mathbf{a}_2})S^{\mathrm{AB}} + b^{\mathrm{U}}_{mn}\Big]\,; \end{aligned} \tag{7}$$

Eq. (3), for $\nu' = b^{\mathrm{D}}_{mn}$:

$$\begin{aligned} a^{\mathrm{D}}_{mn}(1+e^{-i\mathbf{k}\mathbf{a}_1}+e^{i\mathbf{k}\mathbf{a}_2})(\epsilon^{\mathrm{A}}S^{\mathrm{AB}}+T^{\mathrm{AB}}) + b^{\mathrm{D}}_{mn}(\epsilon^{\mathrm{B}}+t^{\mathrm{B}}) \\ = \epsilon_{\mathbf{k}}\Big[a^{\mathrm{D}}_{mn}(1+e^{-i\mathbf{k}\mathbf{a}_1}+e^{i\mathbf{k}\mathbf{a}_2})S^{\mathrm{AB}} + b^{\mathrm{D}}_{mn}\Big]\,; \end{aligned} \tag{8}$$

Note that there is a A/B site specificity in the definition of the nearest-neighbours transfer integral, maintained by the difference in the notation $T^{\mathrm{AB}} \equiv \langle\beta|V_{\mathrm{A}}|\alpha\rangle$ and $T^{\mathrm{BA}} \equiv \langle\beta|V_{\mathrm{B}}|\alpha\rangle$, whereas $S^{\mathrm{AB}} = S^{\mathrm{BA}}$ is obviously symmetric. The "phase factors" depend on the geometry; in our choice of the lattice vectors

$$\mathbf{a}_1 = \frac{a}{2}\left(1,-\sqrt{3}\right)\,; \qquad \mathbf{a}_2 = \frac{a}{2}\left(1,\sqrt{3}\right)\,,$$

$$\begin{aligned} 1+e^{i\mathbf{k}\mathbf{a}_1}+e^{-i\mathbf{k}\mathbf{a}_2} = 1+2\cos\frac{k_x a}{2}e^{-ik_y a\sqrt{3}/2} &\equiv \Delta(\mathbf{k})\,; \\ 1+e^{-i\mathbf{k}\mathbf{a}_1}+e^{+i\mathbf{k}\mathbf{a}_2} = 1+2\cos\frac{k_x a}{2}e^{ik_y a\sqrt{3}/2} &\equiv \Delta^*(\mathbf{k})\,. \end{aligned} \tag{9}$$

We note that the exact choice of phase factors depend on how the outer (anion) planes are organized. The present choice orresponds to the "eclipsed" (wurtzite-like) geometry, as is the case of β and ϵ phases. In hypothetical case of "twisted" anions placement one would need to interchange phase factors at some places.

Ordering the coefficients in all the equations (5) through (8) brings them into a matrix form:

$$\begin{bmatrix} (\epsilon^{\rm A}+t^{\rm A}-\epsilon_{\mathbf{k}}) & \begin{matrix}(\epsilon^{\rm A}S^{\rm AA}+T^{\rm AA}\\ -\epsilon_{\mathbf{k}}S^{\rm AA})\end{matrix} & \begin{matrix}(\epsilon^{\rm B}S^{\rm AB}+T^{\rm BA}\\ -\epsilon_{\mathbf{k}}S^{\rm AB})\Delta(\mathbf{k})\end{matrix} & 0 \\ \begin{matrix}(\epsilon^{\rm A}S^{\rm AA}+T^{\rm AA}\\ -\epsilon_{\mathbf{k}}S^{\rm AA})\end{matrix} & (\epsilon^{\rm A}+t^{\rm A}-\epsilon_{\mathbf{k}}) & 0 & \begin{matrix}(\epsilon^{\rm B}S^{\rm AB}+T^{\rm BA}\\ -\epsilon_{\mathbf{k}}S^{\rm AB})\Delta(\mathbf{k})\end{matrix} \\ \begin{matrix}(\epsilon^{\rm A}S^{\rm AB}+T^{\rm AB}\\ -\epsilon_{\mathbf{k}}S^{\rm AB})\Delta(\mathbf{k})^*\end{matrix} & 0 & (\epsilon^{\rm B}+t^{\rm B}-\epsilon_{\mathbf{k}}) & 0 \\ 0 & \begin{matrix}(\epsilon^{\rm A}S^{\rm AB}+T^{\rm AB}\\ -\epsilon_{\mathbf{k}}S^{\rm AB})\Delta(\mathbf{k})^*\end{matrix} & 0 & (\epsilon^{\rm B}+t^{\rm B}-\epsilon_{\mathbf{k}}) \end{bmatrix} \begin{bmatrix} a^{\rm U}_{mn}(\mathbf{k}) \\ a^{\rm D}_{mn}(\mathbf{k}) \\ b^{\rm U}_{mn}(\mathbf{k}) \\ b^{\rm D}_{mn}(\mathbf{k}) \end{bmatrix} = 0\,, \tag{10}$$

On recasting the parameters as $\epsilon^{\rm A}+t^{\rm A}\rightarrow E^{\rm A}$, $\epsilon^{\rm B}+t^{\rm B}\rightarrow E^{\rm B}$, $\epsilon^{\rm A}S^{\rm AA}+T^{\rm AA}\rightarrow M^{\rm A}$, $\epsilon^{\rm B}S^{\rm BA}+T^{\rm BA}\rightarrow N^{\rm BA}$, $\epsilon^{\rm A}S^{\rm AB}+T^{\rm AB}\rightarrow N^{\rm AB}$, the band energies can be obtained from setting ths determinant to zero:

$$\begin{vmatrix} E^{\rm A}-\epsilon_{\mathbf{k}} & M^{\rm A}-\epsilon_{\mathbf{k}}S^{\rm AA} & (N^{\rm BA}-\epsilon_{\mathbf{k}}S^{\rm AB})\Delta & 0 \\ M^{\rm A}-\epsilon_{\mathbf{k}}S^{\rm AA} & E^{\rm A}-\epsilon_{\mathbf{k}} & 0 & (N^{\rm BA}-\epsilon_{\mathbf{k}}S^{\rm AB})\Delta \\ (N^{\rm AB}-\epsilon_{\mathbf{k}}S^{\rm AB})\Delta^* & 0 & E^{\rm B}-\epsilon_{\mathbf{k}} & 0 \\ 0 & (N^{\rm AB}-\epsilon_{\mathbf{k}}S^{\rm AB})\Delta^* & 0 & E^{\rm B}-\epsilon_{\mathbf{k}} \end{vmatrix} = 0\,, \tag{11}$$

that is, solving the 4th order equation:

$$\begin{aligned} (E^{\rm A}-\epsilon_{\mathbf{k}})^2(E^{\rm B}-\epsilon_{\mathbf{k}})^2-(M^{\rm A}-\epsilon_{\mathbf{k}}S^{\rm AA})^2(E^{\rm B}-\epsilon_{\mathbf{k}})^2 & \\ -2(E^{\rm A}-\epsilon_{\mathbf{k}})(E^{\rm B}-\epsilon_{\mathbf{k}})(N^{\rm AB}-\epsilon_{\mathbf{k}}S^{\rm AB})(N^{\rm BA}-\epsilon_{\mathbf{k}}S^{\rm AB})|\Delta(\mathbf{k})|^2 & \\ +(N^{\rm BA}-\epsilon_{\mathbf{k}}S^{\rm AB})^2(N^{\rm AB}-\epsilon_{\mathbf{k}}S^{\rm AB})^2|\Delta(\mathbf{k})|^4 &= 0\,, \end{aligned} \tag{12}$$

or in the standard form of the quartic equation on $x\equiv\epsilon_{\mathbf{k}}$

$$ax^4+bx^3+cx^2+dx+e=0\,, \qquad \text{with}$$

$$\begin{aligned}
a &= 1-(S^{\mathrm{AA}})^2-2(S^{\mathrm{AB}})^2|\Delta|^2+(S^{\mathrm{AB}})^4|\Delta|^4\,;\\
b &= -2(E^{\mathrm{A}}{+}E^{\mathrm{B}})+2S^{\mathrm{AA}}(M^{\mathrm{A}}{+}E^{\mathrm{B}}S^{\mathrm{AA}})+2S^{\mathrm{AB}}[(E^{\mathrm{A}}{+}E^{\mathrm{B}})S^{\mathrm{AB}}{+}N^{\mathrm{AB}}{+}N^{\mathrm{BA}}]|\Delta|^2\\
&\quad -2(N^{\mathrm{AB}}+N^{\mathrm{BA}})(S^{\mathrm{AB}})^3|\Delta|^4\,;\\
c &= (E^{\mathrm{A}})^2{+}(E^{\mathrm{B}})^2{+}4E^{\mathrm{A}}E^{\mathrm{B}}-(E^{\mathrm{B}})^2(S^{\mathrm{AA}})^2-(M^{\mathrm{A}})^2-4M^{\mathrm{A}}E^{\mathrm{B}}S^{\mathrm{AA}}\\
&\quad -2\left[N^{\mathrm{AB}}N^{\mathrm{BA}}{+}E^{\mathrm{A}}E^{\mathrm{B}}(S^{\mathrm{AB}})^2{+}(E^{\mathrm{A}}{+}E^{\mathrm{B}})S^{\mathrm{AB}}(N^{\mathrm{AB}}{+}N^{\mathrm{BA}})\right]|\Delta|^2\\
&\quad +(S^{\mathrm{AB}})^2\left[(N^{\mathrm{AB}})^2{+}(N^{\mathrm{BA}})^2{+}4N^{\mathrm{AB}}N^{\mathrm{BA}}\right]\,;\\
d &= -2E^{\mathrm{A}}E^{\mathrm{B}}(E^{\mathrm{A}}{+}E^{\mathrm{B}})+M^{\mathrm{A}}S^{\mathrm{AA}}(E^{\mathrm{B}})^2+E^{\mathrm{B}}(M^{\mathrm{A}})^2\\
&\quad +2\left[N^{\mathrm{AB}}N^{\mathrm{BA}}(E^{\mathrm{A}}{+}E^{\mathrm{B}})+S^{\mathrm{AB}}(N^{\mathrm{AB}}{+}N^{\mathrm{BA}})E^{\mathrm{A}}E^{\mathrm{B}}\right]|\Delta|^2\\
&\quad -2N^{\mathrm{AB}}N^{\mathrm{BA}}S^{\mathrm{AB}}(N^{\mathrm{AB}}{+}N^{\mathrm{BA}})|\Delta|^4\,;\\
e &= (E^{\mathrm{A}})^2(E^{\mathrm{B}})^2-(M^{\mathrm{A}})^2(E^{\mathrm{B}})^2-2E^{\mathrm{A}}E^{\mathrm{B}}N^{\mathrm{AB}}N^{\mathrm{BA}}|\Delta|^2\\
&\quad +(N^{\mathrm{AB}})^2(N^{\mathrm{BA}})^2|\Delta|^4\,. \qquad (13)
\end{aligned}$$

The solutions are:

$$\begin{aligned}
(\epsilon_{\mathbf{k}})_1 &= \frac{1}{2}\,\frac{-\boxed{\mathrm{A}}-\boxed{\mathrm{B}}-\sqrt{\boxed{\mathrm{C}}-\boxed{\mathrm{D}}}}{[\,|\Delta|^2(S^{\mathrm{AB}})^2-1]+S^{\mathrm{AA}}}\,, &\quad (\epsilon_{\mathbf{k}})_2 &= \frac{1}{2}\,\frac{\boxed{\mathrm{A}}+\boxed{\mathrm{B}}+\sqrt{\boxed{\mathrm{C}}-\boxed{\mathrm{D}}}}{[\,|\Delta|^2(S^{\mathrm{AB}})^2-1]+S^{\mathrm{AA}}}\,,\\
(\epsilon_{\mathbf{k}})_3 &= \frac{1}{2}\,\frac{-\boxed{\mathrm{A}}+\boxed{\mathrm{B}}-\sqrt{\boxed{\mathrm{C}}+\boxed{\mathrm{D}}}}{[\,|\Delta|^2(S^{\mathrm{AB}})^2-1]-S^{\mathrm{AA}}}\,, &\quad (\epsilon_{\mathbf{k}})_4 &= \frac{1}{2}\,\frac{\boxed{\mathrm{A}}-\boxed{\mathrm{B}}+\sqrt{\boxed{\mathrm{C}}+\boxed{\mathrm{D}}}}{[\,|\Delta|^2(S^{\mathrm{AB}})^2-1]-S^{\mathrm{AA}}}\,, \qquad (14)
\end{aligned}$$

with

$$\boxed{\mathrm{A}} = |\Delta|^2(N^{\mathrm{AB}}+N^{\mathrm{BA}})S^{\mathrm{AB}}-(E^{\mathrm{A}}+E^{\mathrm{B}})\,; \qquad \boxed{\mathrm{B}} = E^{\mathrm{B}}S^{\mathrm{AA}}+M^{\mathrm{A}}\,;$$

$$\begin{aligned}
\boxed{\mathrm{C}} &= |\Delta|^4(N^{\mathrm{AB}}{-}N^{\mathrm{BA}})^2(S^{\mathrm{AB}})^2+4|\Delta|^4E^{\mathrm{A}}E^{\mathrm{B}}(S^{\mathrm{AB}})^2\\
&- 2|\Delta|^2(E^{\mathrm{A}}{+}E^{\mathrm{B}})(N^{\mathrm{AB}}{+}N^{\mathrm{BA}})S^{\mathrm{AB}}+(E^{\mathrm{B}})^2(S^{\mathrm{AA}})^2-2E^{\mathrm{B}}M^{\mathrm{A}}S^{\mathrm{AA}}\\
&+ 4|\Delta|^2N^{\mathrm{AB}}N^{\mathrm{BA}}+(M^{\mathrm{A}})^2+(E^{\mathrm{B}}{-}E^{\mathrm{A}})^2\,; \qquad (15)
\end{aligned}$$

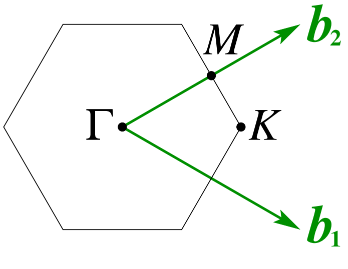
$$\begin{aligned}
\boxed{\mathrm{D}} &= 4|\Delta|^2E^{\mathrm{B}}M^{\mathrm{A}}(S^{\mathrm{AB}})^2-2|\Delta|^2E^{\mathrm{B}}(N^{\mathrm{AB}}{+}N^{\mathrm{BA}})S^{\mathrm{AA}}\\
&- 2|\Delta|^2M^{\mathrm{A}}(N^{\mathrm{AB}}{+}N^{\mathrm{BA}})S^{\mathrm{AB}}+4|\Delta|^2N^{\mathrm{AB}}N^{\mathrm{BA}}S^{\mathrm{AA}}+2(E^{\mathrm{B}})^2S^{\mathrm{AA}}\\
&- 2E^{\mathrm{A}}E^{\mathrm{B}}S^{\mathrm{AA}}-2M^{\mathrm{A}}(E^{\mathrm{B}}{-}E^{\mathrm{A}})\,. \qquad (16)
\end{aligned}$$

For the translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$ as specified above, the reciprocal vectors are

$$\mathbf{b}_1 = \frac{2\pi}{a}\left(1,-\frac{1}{\sqrt{3}}\right)\,; \qquad \mathbf{b}_2 = \frac{2\pi}{a}\left(1,\frac{1}{\sqrt{3}}\right)\,,$$

and the symmetry points of the Brillouin zone have the coordinates:

$$M = \frac{\pi}{a}\left(1,\frac{1}{\sqrt{3}}\right)\,; \qquad K = \frac{2\pi}{a}\left(\frac{2}{3},0\right)\,.$$



The values of $\Delta(\mathbf{k})$ at the symmetry points are:

$$\Delta(\Gamma) = 3\,; \qquad \Delta(M) = 1\,; \qquad \Delta(K) = 0\,.$$

For K, the solution is straightforward; the four band energies are:

$$\epsilon_{\mathbf{k}=K} = \left\{\, E^{\mathrm{B}}\,; \quad E^{\mathrm{B}}\,; \quad \frac{E^{\mathrm{A}} - M^{\mathrm{A}}}{1 - S^{\mathrm{AA}}}\,; \quad \frac{E^{\mathrm{A}} + M^{\mathrm{A}}}{1 + S^{\mathrm{AA}}} \,\right\}\,.$$