Two-dimensional bilayer blue phosphorus Dirac-like material: A multi-orbital tight-binding investigation

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Electronic dispersion derivation in the presence of various neighbors within the MOTB model.

In this section, we provide slightly additional details of the derivations of dispersion relations in the presence of various NN within the MOTB model. With regard to the B_0 central atom, the lattice displacement vectors of the first (A_{1j}, j = 1–3), second (B_{2j}, j = 1–6), third (A_{3j}, j = 1–3), fourth (A_{4j}, j = 1–6), and fifth nearest-neighbors (B_{5j}, j = 1–6) are defined respectively as:

$\vec{d_{1j}} = \tau_{A1j} - \tau_{B0}, \vec{d_{2j}} = \tau_{B2j} - \tau_{B0}, \vec{d_{3j}} = \tau_{A3j} - \tau_{B0}, \vec{d_{4j}} = \tau_{A4j} - \tau_{B0}, \vec{d_{5j}} = \tau_{B5j} - \tau_{B0}.$

Where $\boldsymbol{\tau}$ is the atomic position (A_{1j} an atom in sublattice A at a given site). In the case of monolayer and within the NN interaction MOTB approximation, the different coupling matrix elements hopping integrals are presented:

$$\varepsilon_s = \int \phi_s^*(\vec{r} - \vec{\tau_{B0}})\hat{H}\phi_s(\vec{r} - \vec{\tau_{B0}})d^3r = \langle \phi_{s,B0} \,|\, H \,|\, \phi_{s,B0} \rangle, \tag{A.1}$$

$$\varepsilon_p = \int \phi_p^*(\vec{r} - \vec{\tau_{B0}})\hat{H}\phi_p(\vec{r} - \vec{\tau_{B0}})d^3r = \langle \phi_{p,B0} \,|\, H \,|\, \phi_{p,B0} \rangle, \tag{A.2}$$

$$V_{ss\sigma} = \int \phi_s^*(\vec{r} - \vec{\tau_{B0}})\hat{H}\phi_s(\vec{r} - \vec{\tau_{A1j}})d^3r = \langle \phi_{s,B0} \,|\, H \,|\, \phi_{s,A1j} \rangle, \tag{A.3}$$

$$V_{sp\sigma} = \int \phi_s^*(\vec{r} - \vec{\tau_{B0}})\hat{H}\phi_p(\vec{r} - \vec{\tau_{A1j}})d^3r = \langle \phi_{s,B0} \,|\, H \,|\, \phi_{p,A1j} \rangle, \tag{A.4}$$

$$V_{pp\sigma} = \int \phi_p^*(\vec{r} - \vec{\tau_{B0}})\hat{H}\phi_p(\vec{r} - \vec{\tau_{A1j}})d^3r = \langle \phi_{p,B0} \,|\, H \,|\, \phi_{p,A1j} \rangle, \tag{A.5}$$

$$V_{pp\pi} = \int \phi_p^*(\vec{r} - \vec{\tau_{B0}})\hat{H}\phi_p(\vec{r} - \vec{\tau_{A1j}})d^3r = \langle \phi_{p,B0} \,|\, H \,|\, \phi_{p,A1j} \rangle, \tag{A.6}$$

$$S_{ss} = \int \phi_s^*(\vec{r} - \vec{\tau_{B0}})\phi_s(\vec{r} - \vec{\tau_{B0}})d^3r = \langle \phi_{s,B0} \,|\, \phi_{s,B0} \rangle = 1, \tag{A.7}$$

$$S_{ss} = \int \phi_s^*(\vec{r} - \vec{\tau_{B0}})\phi_s(\vec{r} - \vec{\tau_{A1j}})d^3r = \langle \phi_{s,B0} \,|\, \phi_{s,A1j} \rangle = 0, \tag{A.8}$$

$$\begin{aligned}\Psi_{\vec{k}}(\vec{r}) &= c_{s,m}(\vec{k})\psi_{s,m,\vec{k}}(\vec{r}) + c_{x,m}(\vec{k})\psi_{x,m,\vec{k}}(\vec{r}) + c_{y,m}(\vec{k})\psi_{y,m,\vec{k}}(\vec{r}) + c_{z,m}(\vec{k})\psi_{z,m,\vec{k}}(\vec{r}) \\ &= 1/\sqrt{N}\Big[e^{i\vec{k}\vec{\tau_{B0}}}\big(c_{s,B0}\phi_s(\vec{r} - \vec{\tau_{B0}}) + c_{x,B0}\phi_x(\vec{r} - \vec{\tau_{B0}}) + c_{y,B0}\phi_y(\vec{r} - \vec{\tau_{B0}}) + c_{z,B0}\phi \\ &,\end{aligned} \tag{A.9}$$

$$\langle \Psi_{\vec{k}}(\vec{r}) \,|\, H \,|\, \Psi_{\vec{k}}(\vec{r}) \rangle = E\langle \Psi_{\vec{k}}(\vec{r}) \,|\, \Psi_{\vec{k}}(\vec{r}) \rangle, \tag{A.10}$$

The r.h.s of the equation (A.10):

$$\begin{aligned}&\int \Big(1/\sqrt{N}\sum_r^N e^{-i\vec{k}\vec{R}_r}\Big[e^{-i\vec{k}\vec{\tau_{B0}}}\big(\phi_s^*(\vec{r} - \vec{\tau_{B0}})\big)\Big]\Big)\hat{H}\Big(1/\sqrt{N}\sum_u^N e^{i\vec{k}\vec{R}_u}\Big[e^{i\vec{k}\vec{\tau_{B0}}}\big(c_{s,B0}\phi_s(\vec{r} - \\ &d^3r = \int 1/N\sum_r^N\sum_u^N e^{i\vec{k}(\vec{R}_u - \vec{R}_r)}\Big[e^{-i\vec{k}\vec{\tau_{B0}}}\big(\phi_s^*(\vec{r} - \vec{\tau_{B0}})\big)\hat{H}\Psi_{\vec{k}}(\vec{r})\Big]d^3r,\end{aligned} \tag{A.11}$$

The l.h.s of the equation (A.10):

$$E \int \left(1/\sqrt{N}\sum_{r}^{N} e^{-i\vec{k}\vec{R}_r}\left[e^{-i\vec{k}\vec{\tau}_{B0}}\left(\phi_s^*\left(\vec{r}-\vec{\tau}_{B0}\right)\right)\right]\right)\left(1/\sqrt{N}\sum_{u}^{N} e^{i\vec{k}\vec{R}_u}\left[e^{i\vec{k}\vec{\tau}_{B0}}\left(c_{s,B0}\phi_s\left(\vec{r}-\tau\right.\right.\right.\right.$$
$$d^3r = E\int 1/N\sum_{r}^{N}\sum_{u}^{N} e^{i\vec{k}\left(\vec{R}_u-\vec{R}_r\right)}\left[e^{-i\vec{k}\vec{\tau}_{B0}}\left(\phi_s^*\left(\vec{r}-\vec{\tau}_{B0}\right)\right)\Psi_{\vec{k}}(\vec{r})\right]d^3r, \tag{A.12}$$

Which leads to the secular equation:

$$\begin{pmatrix}
 & s_B & x_B & y_B & z_B & s_A & x_A & y_A & z_A \\
s_B^* & \varepsilon_s - E(k) & 0 & 0 & 0 & E_{ss}^{(11)} g_{s1} & E_{sx}^{(13)} g_{1312}^{-} & E_{sy}^{(11)} g_{11}^{+} + E_{sy}^{(13)} g_{1312}^{+} & E_{sz}^{(11)} g_{s1} \\
x_B^* & 0 & \varepsilon_x - E(k) & 0 & 0 & -E_{sx}^{(13)} g_{1312}^{-} & E_{xx}^{(11)} g_{11}^{+} + E_{xx}^{(13)} g_{1312}^{+} & E_{xy}^{(12)} g_{1213}^{-} & E_{xz}^{(13)} g_{1312}^{-} \\
y_B^* & 0 & 0 & \varepsilon_y - E(k) & 0 & -E_{sy}^{(11)} g_{11}^{+} - E_{sy}^{(13)} g_{1312}^{+} & E_{xy}^{(12)} g_{1213}^{-} & E_{yy}^{(11)} g_{11}^{+} + E_{yy}^{(13)} g_{1312}^{+} & E_{yz}^{(11)} g_{11}^{+} + E_{yz}^{(13)} g_{1312}^{+} \\
z_B^* & 0 & 0 & 0 & \varepsilon_z - E(k) & -E_{sz}^{(11)} g_{s1} & E_{xz}^{(13)} g_{1312}^{-} & E_{yz}^{(11)} g_{11}^{+} + E_{yz}^{(13)} g_{1312}^{+} & E_{zz}^{(11)} g_{s1} \\
s_A^* & E_{ss}^{(11)} g_{s1}^{*} & -E_{sx}^{(13)} g_{1312}^{-*} & -E_{sy}^{(11)} g_{11}^{+*} - E_{sy}^{(13)} g_{1312}^{+*} & -E_{sz}^{(11)} g_{s1}^{*} & \varepsilon_s - E(k) & 0 & 0 & 0 \\
x_A^* & E_{sx}^{(13)} g_{1312}^{-*} & E_{xx}^{(11)} g_{11}^{+*} + E_{xx}^{(13)} g_{1312}^{+*} & E_{xy}^{(12)} g_{1213}^{-*} & E_{xz}^{(13)} g_{1312}^{-*} & 0 & \varepsilon_x - E(k) & 0 & 0 \\
y_A^* & E_{sy}^{(11)} g_{11}^{+*} + E_{sy}^{(13)} g_{1312}^{+*} & E_{xy}^{(12)} g_{1213}^{-*} & E_{yy}^{(11)} g_{11}^{+*} + E_{yy}^{(13)} g_{1312}^{+*} & E_{yz}^{(11)} g_{11}^{+*} + E_{yz}^{(13)} g_{1312}^{+*} & 0 & 0 & \varepsilon_y - E(k) & 0 \\
z_A^* & E_{sz}^{(11)} g_{s1}^{*} & E_{xz}^{(13)} g_{1312}^{-*} & E_{yz}^{(11)} g_{11}^{+*} + E_{yz}^{(13)} g_{1312}^{+*} & E_{zz}^{(11)} g_{s1}^{*} & 0 & 0 & 0 & \varepsilon_z - E(k)
\end{pmatrix},$$

Note that solving the Hamiltonian matrix can be accomplished using Matlab, Python, Mathematica, GNU Octave, Fortran, Spark or Julia. This is sufficient to show how the other matrix elements are evaluated. Based on the atomic positions, we define the different displacement vectors and SK parameters, from 11 (NN with bond orientation number 1) to 56 (5NN with bond orientation number 6) as previously mentioned (see Fig. 1).

With:

$$M_0 = \begin{pmatrix} \varepsilon_s & 0 & 0 & 0 \\ 0 & \varepsilon_x & 0 & 0 \\ 0 & 0 & \varepsilon_y & 0 \\ 0 & 0 & 0 & \varepsilon_z \end{pmatrix}, \tag{A.13}$$

$$M_1 = \begin{pmatrix} E_{ss}^{(11)} g_{s1} & E_{sx}^{(13)} g_{1312}^{-} & E_{sy}^{(11)} g_{11}^{+} + E_{sy}^{(13)} g_{1312}^{+} & E_{sz}^{(11)} g_{s1} \\ -E_{sx}^{(13)} g_{1312}^{-} & E_{xx}^{(11)} g_{11}^{+} + E_{xx}^{(13)} g_{1312}^{+} & E_{xy}^{(12)} g_{1213}^{-} & E_{xz}^{(13)} g_{1312}^{-} \\ -E_{sy}^{(11)} g_{11}^{+} - E_{sy}^{(13)} g_{1312}^{+} & E_{xy}^{(12)} g_{1213}^{-} & E_{yy}^{(11)} g_{11}^{+} + E_{yy}^{(13)} g_{1312}^{+} & E_{yz}^{(11)} g_{11}^{+} + E_{yz}^{(13)} g_{1312}^{+} \\ -E_{sz}^{(11)} g_{s1} & E_{xz}^{(13)} g_{1312}^{-} & E_{yz}^{(11)} g_{11}^{+} + E_{yz}^{(13)} g_{1312}^{+} & E_{zz}^{(11)} g_{s1} \end{pmatrix}, \tag{A.14}$$

Where the phase factors and SK parameters are expressed as follows:

$$g_{1j}^{+} = exp\left(i\vec{k}\vec{d}_{1j}\right),\ g_{s1} = \sum_{j=1}^{3} exp\left(i\vec{k}\vec{d}_{1j}\right),\ g_{1312}^{\pm} = exp\left(i\vec{k}\vec{d}_{13}\right) \pm exp\left(i\vec{k}\vec{d}_{12}\right),\ g_{1213}^{-} = exp\left(i\vec{k}\vec{d}_{12}\right) - exp\left(i\vec{k}\vec{d}_{13}\right), \tag{A.15}$$

$$E_{ss}^{nj} = V_{ss\sigma}(d_{nj}),\ E_{s\alpha}^{nj} = \left(d_{\alpha}^{nj}/d_{nj}\right)V_{sp\sigma}(d_{nj}),\ E_{\alpha\beta}^{nj} = \left(d_{\alpha}^{nj}d_{\beta}^{nj}/d_{nj}^{2}\right)V_{pp\sigma}(d_{nj}) + \left(\delta_{\alpha\beta} - \left(d_{\alpha}^{nj}d_{\beta}^{nj}/d_{nj}^{2}\right)\right)V_{pp\pi}(d_{nj}),\ \alpha,\beta = x, y, z. \tag{A.16}$$

$$M_2 = \begin{pmatrix} E_{ss}^{(21)} g_{s2} & E_{sx}^{(21)} g_{2126} + E_{sx}^{(23)} g_{2324}^{-} & E_{sy}^{(21)} g_{2126}^{-} & 0 \\ -E_{sx}^{(21)} g_{2126} - E_{sx}^{(23)} g_{2324}^{-} & E_{xx}^{(21)} g_{2126}^{+} + E_{xx}^{(23)} g_{2324}^{+} & E_{xy}^{(21)} g_{2126}^{--} & 0 \\ -E_{sy}^{(21)} g_{2126}^{-} & E_{xy}^{(21)} g_{2126}^{--} & E_{yy}^{(21)} g_{2126}^{+} + E_{yy}^{(23)} g_{2324}^{+} & 0 \\ 0 & 0 & 0 & E_{zz}^{(21)} g_{s2} \end{pmatrix}, \tag{A.17}$$

$$\begin{aligned} g_{2126} &= exp\left(i\vec{k}\vec{d}_{21}\right) - exp\left(i\vec{k}\vec{d}_{22}\right) + exp\left(i\vec{k}\vec{d}_{25}\right) - exp\left(i\vec{k}\vec{d}_{26}\right),\ g_{2324}^{\pm} = exp\left(i\vec{k}\vec{d}_{23}\right) \pm \\ & exp\left(i\vec{k}\vec{d}_{26}\right),\ g_{2126}^{+} \\ &= exp\left(i\vec{k}\vec{d}_{21}\right) + exp\left(i\vec{k}\vec{d}_{22}\right) + exp\left(i\vec{k}\vec{d}_{25}\right) + exp\left(i\vec{k}\vec{d}_{26}\right),\ g_{2126}^{--} = exp\left(i\vec{k}\vec{d}_{21}\right) - \\ &= \sum_{j=1}^{6} exp\left(i\vec{k}\vec{d}_{2j}\right), \end{aligned} \tag{A.18}$$

Note that from here onward, we consider that the transfer parameter exponentially depends on the vector positions d_{nj}:

$$M_3 = \begin{pmatrix} E_{ss}^{(31)} g_{s3} & E_{sx}^{(31)} g_{3132}^{-} & E_{sy}^{(31)} g_{3132}^{+} + E_{sy}^{(33)} g_{33}^{+} & E_{sz}^{(31)} g_{s3} \\ -E_{sx}^{(31)} g_{3132}^{-} & E_{xx}^{(31)} g_{3132}^{+} + E_{xx}^{(33)} g_{33}^{+} & E_{xy}^{(31)} g_{3132}^{-} & E_{xz}^{(31)} g_{3132}^{-} \\ -E_{sy}^{(31)} g_{3132}^{+} - E_{sy}^{(33)} g_{33}^{+} & E_{xy}^{(31)} g_{3132}^{-} & E_{yy}^{(31)} g_{3132}^{+} + E_{yy}^{(33)} g_{33}^{+} & E_{yz}^{(31)} g_{3132}^{+} + E_{yz}^{(33)} g_{33}^{+} \\ -E_{sz}^{(31)} g_{s3} & E_{xz}^{(31)} g_{3132}^{-} & E_{yz}^{(31)} g_{3132}^{+} + E_{yz}^{(33)} g_{33}^{+} & E_{zz}^{(31)} g_{s3} \end{pmatrix}, \tag{A.19}$$

$$g_{3j}^{+} = exp\left(i\vec{k}\vec{d}_{3j}\right),\ g_{3132}^{\pm} = exp\left(i\vec{k}\vec{d}_{31}\right) \pm exp\left(i\vec{k}\vec{d}_{32}\right),\ g_{s3} = \sum_{j=1}^{3} exp\left(i\vec{k}\vec{d}_{3j}\right), \tag{A.20}$$

$$M_4 = \begin{pmatrix} E_{ss}^{(41)} g_{s4} & E_{sx}^{(41)} g_{4142}^{-} + E_{sx}^{(43)} g_{4344}^{-} + E_{sx}^{(45)} g_{4546}^{-} & E_{sy}^{(41)} g_{4142}^{+} + E_{sy}^{(43)} g_{4344}^{+} + E_{sy}^{(45)} g_{4546}^{+} & E_{sz}^{(41)} g_{s4} \\ -E_{sx}^{(41)} g_{4142}^{-} - E_{sx}^{(43)} g_{4344}^{-} - E_{sx}^{(45)} g_{4546}^{-} & E_{xx}^{(41)} g_{4142}^{+} + E_{xx}^{(43)} g_{4344}^{+} + E_{xx}^{(45)} g_{4546}^{+} & E_{xy}^{(41)} g_{4142}^{-} + E_{xy}^{(44)} g_{4344}^{--} + E_{xy}^{(46)} g_{4546}^{--} & E_{xz}^{(41)} g_{4142}^{-} + E_{xz}^{(43)} g_{4344}^{-} + E_{xz}^{(45)} g_{4546}^{-} \\ -E_{sy}^{(41)} g_{4142}^{+} - E_{sy}^{(43)} g_{4344}^{+} - E_{sy}^{(45)} g_{4546}^{+} & E_{xy}^{(41)} g_{4142}^{-} + E_{xy}^{(44)} g_{4344}^{--} + E_{xy}^{(46)} g_{4546}^{--} & E_{yy}^{(41)} g_{4142}^{+} + E_{yy}^{(43)} g_{4344}^{+} + E_{yy}^{(45)} g_{4546}^{+} & E_{yz}^{(41)} g_{4142}^{+} + E_{yz}^{(43)} g_{4344}^{+} + E_{yz}^{(45)} g_{4546}^{+} \\ -E_{sz}^{(41)} g_{s4} & E_{xz}^{(41)} g_{4142}^{-} + E_{xz}^{(43)} g_{4344}^{-} + E_{xz}^{(45)} g_{4546}^{-} & E_{yz}^{(41)} g_{4142}^{+} + E_{yz}^{(43)} g_{4344}^{+} + E_{yz}^{(45)} g_{4546}^{+} & E_{zz}^{(41)} g_{s4} \end{pmatrix} \quad (A.21)$$

$$g_{4142}^{\pm} = exp(i\vec{k}\vec{d}_{41}) \pm exp(i\vec{k}\vec{d}_{42}),\ g_{4344}^{\pm} = exp(i\vec{k}\vec{d}_{43}) \pm exp(i\vec{k}\vec{d}_{44}),\ g_{4546}^{\pm} = exp(i\vec{k} \quad (A.22)$$
$$exp(i\vec{k}\vec{d}_{46}) - exp(i\vec{k}\vec{d}_{45}),\ g_{s4} = \sum_{j=1}^{6} exp(i\vec{k}\vec{d}_{4j}),$$

$$M_5 = \begin{pmatrix} E_{ss}^{(51)} g_{s5} & E_{sx}^{(52)} g_{5256}^{-} & E_{sy}^{(51)} g_{5155}^{-} + E_{sy}^{(52)} g_{5256}^{--} & 0 \\ -E_{sx}^{(52)} g_{5256}^{-} & E_{xx}^{(51)} g_{5155}^{+} + E_{xx}^{(52)} g_{5256}^{+} & E_{xy}^{(52)} g_{5256}^{---} & 0 \\ -E_{sy}^{(51)} g_{5155}^{-} - E_{sy}^{(52)} g_{5256}^{--} & E_{xy}^{(52)} g_{5256}^{---} & E_{yy}^{(51)} g_{5155}^{+} + E_{yy}^{(52)} g_{5256}^{+} & 0 \\ 0 & 0 & 0 & E_{zz}^{(51)} g_{s5} \end{pmatrix}, \quad (A.23)$$

$$g_{5256}^{--} = exp(i\vec{k}\vec{d}_{52}) + exp(i\vec{k}\vec{d}_{53}) - exp(i\vec{k}\vec{d}_{54}) - exp(i\vec{k}\vec{d}_{56}),\ g_{5155}^{\pm} = exp(i\vec{k}\vec{d}_{51}) \pm$$
$$exp(i\vec{k}\vec{d}_{56}),\ g_{5256}^{+} = exp(i\vec{k}\vec{d}_{52}) + exp(i\vec{k}\vec{d}_{53}) + exp(i\vec{k}\vec{d}_{54}) + exp(i\vec{k}\vec{d}_{56}),\ g_{5256}^{---} = exp(i\vec{k}\vec{d}_{52}) - \quad (A.24)$$
$$= \sum_{j=1}^{6} exp(i\vec{k}\vec{d}_{5j}),$$

$$M_{zeros} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (A.25)$$

$$M_{2'} = \begin{pmatrix} E_{ss}^{(11')} & 0 & 0 & E_{sz}^{(11')} \\ 0 & E_{xx}^{(11')} & 0 & 0 \\ 0 & 0 & E_{yy}^{(11')} & 0 \\ -E_{sz}^{(11')} & 0 & 0 & E_{zz}^{(11')} \end{pmatrix}, \quad (A.26)$$

$$M_{3'} = \begin{pmatrix} E_{ss}^{(11')} g_{s1'} & E_{sx}^{(13')} g_{1312'}^{-} & E_{sy}^{(11')} g_{11'}^{+} + E_{sy}^{(13')} g_{1312'}^{+} & E_{sz}^{(11')} g_{s1'} \\ -E_{sx}^{(13')} g_{1312'}^{-} & E_{xx}^{(11')} g_{11'}^{+} + E_{xx}^{(13')} g_{1312'}^{+} & E_{xy}^{(12')} g_{1213'}^{-} & E_{xz}^{(13')} g_{1312'}^{-} \\ -E_{sy}^{(11')} g_{11'}^{+} - E_{sy}^{(13')} g_{1312'}^{+} & E_{xy}^{(12')} g_{1213'}^{-} & E_{yy}^{(11')} g_{11'}^{+} + E_{yy}^{(13')} g_{1312'}^{+} & E_{yz}^{(11')} g_{11'}^{+} + E_{yz}^{(13')} g_{1312'}^{+} \\ -E_{sz}^{(11')} g_{s1'} & E_{xz}^{(13')} g_{1312'}^{-} & E_{yz}^{(11')} g_{11'}^{+} + E_{yz}^{(13')} g_{1312'}^{+} & E_{zz}^{(11')} g_{s1'} \end{pmatrix}, \quad (A.27)$$

$$g_{s1'} = \sum_{j=1}^{3} exp(i\vec{k}\vec{d}_{1j'}),\ g_{1312'}^{\pm} = exp(i\vec{k}\vec{d}_{13'}) \pm exp(i\vec{k}\vec{d}_{12'}),\ g_{1213'}^{-} = exp(i\vec{k}\vec{d}_{12'}) - exp(i\vec{k}\vec{d}_{13'}), \quad (A.28)$$

$$M_{5'} = \begin{pmatrix} E_{ss}^{(21')} & 0 & 0 & E_{sz}^{(21')} \\ 0 & E_{xx}^{(21')} & 0 & 0 \\ 0 & 0 & E_{yy}^{(21')} & 0 \\ -E_{sz}^{(21')} & 0 & 0 & E_{zz}^{(21')} \end{pmatrix}, \quad (A.29)$$

AA stacking within the 5NN in- and 2NN out-of-plane coupling MOTB approach (A.25)–(A.29).

TABLE I. Structural parameters of the strained AA stacked bilayer buk-P.

	a (Å)	***Δ_{int}*** (Å)	***h_{BA}*** (Å)	***b*** (Å)	***E_g*** (meV)
AA stacked bilayer form	4.70	2.14	0	2.7	400
	4.60	2.24	0	2.66	310
	4.34	2.07	0.16	2.51	280
	4.26	2.09	0.10	2.46	280
	4.20	2.20	0	2.42	270
	4.00	2.602	0.045	2.31	1

Matlab code of the monolayer buk-P within the 5NN intralayer coupling MOTB model:

```
%-----------Programmed by: BENHAIJ Amine-----------------------%

%--------------------------------------------------------------%

%------------------------About--------------------------------%
% It calculates the energy band structure of monolayer blue
% Phosphorene using a (MOTB) approach including up to the fifth
% nearest neighbor in-plane couplings
%--------------------------------------------------------------%
clear variables;
close all;
clc;
%--------------------------------------------------------------%

%-------------Crystal structure and Brillouin zone--------------%
a = 3.28;  %Lattice constant |Angstrom|

d_vertical = 1.23;  %Vertical distance between A and B |Angstrom|
%--------------------------------------------------------------%

%-------------Coordinates of atoms------------------------------%
tau_B_center = [0, 0, 0];
%--------------------------------------------------------------%

tau_A_1_1 = [0, a/sqrt(3), d_vertical];
tau_A_1_2 = [a/2, -a/2/sqrt(3), d_vertical];
tau_A_1_3 = [-a/2, -a/2/sqrt(3), d_vertical];
%--------------------------------------------------------------%

tau_B_2_1 = [a/2, (3*a)/2/sqrt(3), 0];
tau_B_2_2 = [-a/2, (3*a)/2/sqrt(3), 0];
tau_B_2_3 = [a, 0, 0];
tau_B_2_4 = [-a, 0, 0];
tau_B_2_5 = [a/2, -(3*a)/2/sqrt(3), 0];
tau_B_2_6 = [-a/2, -(3*a)/2/sqrt(3), 0];
%--------------------------------------------------------------%

tau_A_3_1 = [a, a/sqrt(3), d_vertical];
tau_A_3_2 = [-a, a/sqrt(3), d_vertical];
tau_A_3_3 = [0, -(2*a)/sqrt(3), d_vertical];
%--------------------------------------------------------------%

tau_A_4_1 = [a/2, (5*a)/2/sqrt(3), d_vertical];
tau_A_4_2 = [-a/2, (5*a)/2/sqrt(3), d_vertical];
tau_A_4_3 = [(3*a)/2, -a/2/sqrt(3), d_vertical];
tau_A_4_4 = [-(3*a)/2, -a/2/sqrt(3), d_vertical];
tau_A_4_5 = [a, -(2*a)/sqrt(3), d_vertical];
tau_A_4_6 = [-a, -(2*a)/sqrt(3), d_vertical];
%--------------------------------------------------------------%

tau_B_5_1 = [0, (3*a)/sqrt(3), 0];
tau_B_5_2 = [(3*a)/2, (3*a)/2/sqrt(3), 0];
tau_B_5_3 = [-(3*a)/2, (3*a)/2/sqrt(3), 0];
tau_B_5_4 = [(3*a)/2, -(3*a)/2/sqrt(3), 0];
tau_B_5_5 = [0, -(3*a)/sqrt(3), 0];
tau_B_5_6 = [-(3*a)/2, -(3*a)/2/sqrt(3), 0];
%--------------------------------------------------------------%

%--------Brillouin zone High symmetry points of k-space---------%
gamma = [0, 0];
K = [(2 * pi)/(3 * a), (2 * pi)/(sqrt(3) * a)];
M = [0, (2 * pi)/(sqrt(3) * a)];  %#ok<*NASGU>
%--------------------------------------------------------------%

%-------------Lattice displacement vectors----------------------%
d_1 = tau_A_1_1 - tau_B_center;
x_d_1 = d_1(:,1);
y_d_1 = d_1(:,2);
z_d_1 = d_1(:,3);

d_2 = tau_A_1_3 - tau_B_center;
x_d_2 = d_2(:,1);
y_d_2 = d_2(:,2);
z_d_2 = d_2(:,3);

d_3 = tau_A_1_2 - tau_B_center;
x_d_3 = d_3(:,1);
y_d_3 = d_3(:,2);
z_d_3 = d_3(:,3);

distance_1 = sqrt((x_d_1)^2 + (y_d_1)^2 + (z_d_1)^2); %Distance between atom
A and B |Angstrom|
%--------------------------------------------------------------%

d_4 = tau_B_2_1 - tau_B_center;
x_d_4 = d_4(:,1);
y_d_4 = d_4(:,2);
z_d_4 = d_4(:,3);

d_5 = tau_B_2_2 - tau_B_center;
x_d_5 = d_5(:,1);
y_d_5 = d_5(:,2);
z_d_5 = d_5(:,3);

d_6 = tau_B_2_3 - tau_B_center;
x_d_6 = d_6(:,1);
y_d_6 = d_6(:,2);
z_d_6 = d_6(:,3);

d_7 = tau_B_2_4 - tau_B_center;
x_d_7 = d_7(:,1);
y_d_7 = d_7(:,2);
z_d_7 = d_7(:,3);

d_8 = tau_B_2_5 - tau_B_center;
x_d_8 = d_8(:,1);
y_d_8 = d_8(:,2);
z_d_8 = d_8(:,3);

d_9 = tau_B_2_6 - tau_B_center;
x_d_9 = d_9(:,1);
y_d_9 = d_9(:,2);
z_d_9 = d_9(:,3);

distance_2 = sqrt((x_d_4)^2 + (y_d_4)^2 + (z_d_4)^2); %Distance between atom
B and B |Angstrom|
%--------------------------------------------------------------%

d_10 = tau_A_3_1 - tau_B_center;
x_d_10 = d_10(:,1);
y_d_10 = d_10(:,2);
z_d_10 = d_10(:,3);

d_11 = tau_A_3_2 - tau_B_center;
x_d_11 = d_11(:,1);
y_d_11 = d_11(:,2);
z_d_11 = d_11(:,3);

d_12 = tau_A_3_3 - tau_B_center;
x_d_12 = d_12(:,1);
y_d_12 = d_12(:,2);
z_d_12 = d_12(:,3);

distance_3 = sqrt((x_d_10)^2 + (y_d_10)^2 + (z_d_10)^2); %Distance between
atom B and A 3rd (nn) |Angstrom|
%--------------------------------------------------------------%

d_13 = tau_A_4_1 - tau_B_center;
x_d_13 = d_13(:,1);
y_d_13 = d_13(:,2);
z_d_13 = d_13(:,3);

d_14 = tau_A_4_2 - tau_B_center;
x_d_14 = d_14(:,1);
y_d_14 = d_14(:,2);
z_d_14 = d_14(:,3);

d_15 = tau_A_4_3 - tau_B_center;
x_d_15 = d_15(:,1);
y_d_15 = d_15(:,2);
z_d_15 = d_15(:,3);

d_16 = tau_A_4_4 - tau_B_center;
x_d_16 = d_16(:,1);
y_d_16 = d_16(:,2);
z_d_16 = d_16(:,3);

d_17 = tau_A_4_5 - tau_B_center;
x_d_17 = d_17(:,1);
y_d_17 = d_17(:,2);
z_d_17 = d_17(:,3);

d_18 = tau_A_4_6 - tau_B_center;
x_d_18 = d_18(:,1);
y_d_18 = d_18(:,2);
z_d_18 = d_18(:,3);

distance_4 = sqrt((x_d_13)^2 + (y_d_13)^2 + (z_d_13)^2); %Distance between
atom B and A 4th (nn) |Angstrom|
%--------------------------------------------------------------%

d_19 = tau_B_5_1 - tau_B_center;
x_d_19 = d_19(:,1);
y_d_19 = d_19(:,2);
z_d_19 = d_19(:,3);

d_20 = tau_B_5_2 - tau_B_center;
x_d_20 = d_20(:,1);
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y_d_20 = d_20(:,2);
z_d_20 = d_20(:,3);

d_21 = tau_B_5_3 - tau_B_center;
x_d_21 = d_21(:,1);
y_d_21 = d_21(:,2);
z_d_21 = d_21(:,3);

d_22 = tau_B_5_4 - tau_B_center;
x_d_22 = d_22(:,1);
y_d_22 = d_22(:,2);
z_d_22 = d_22(:,3);

d_23 = tau_B_5_5 - tau_B_center;
x_d_23 = d_23(:,1);
y_d_23 = d_23(:,2);
z_d_23 = d_23(:,3);

d_24 = tau_B_5_6 - tau_B_center;
x_d_24 = d_24(:,1);
y_d_24 = d_24(:,2);
z_d_24 = d_24(:,3);

distance_5 = sqrt((x_d_19)^2 + (y_d_19)^2 + (z_d_19)^2); %Distance between atom B and B 5th (nn) |Angstrom|
%---------------------------------------------------------------%

%-------------Hamiltonian SK parameters-------------------------%

%-------------All the SK parameters are in eV-------------------%
Epsilon_s = -8.55;
Epsilon_p_x = -4.0;
Epsilon_p_y = -4.0;
Epsilon_p_z = -4.0;
%---------------------------------------------------------------%

V_s_s_sigma_1 = -1.0;
V_s_p_sigma_1 = -2.90;
V_p_p_sigma_1 = 3.30;
V_p_p_pi_1 = -0.70;

V_s_s_sigma_2 = -1.0;
V_s_p_sigma_2 = -2.90;
V_p_p_sigma_2 = 3.30;
V_p_p_pi_2 = -0.70;

V_s_s_sigma_3 = -1.0;
V_s_p_sigma_3 = -2.90;
V_p_p_sigma_3 = 3.30;
V_p_p_pi_3 = -0.70;
%---------------------------------------------------------------%

decay_r_2 = 1;

V_s_s_sigma_4 =  0.25 * decay_r_2;
V_s_p_sigma_4 = -0.30 * decay_r_2;
V_p_p_sigma_4 =  1.15 * decay_r_2;
V_p_p_pi_4 =    -0.40 * decay_r_2;

V_s_s_sigma_5 = V_s_s_sigma_4 * decay_r_2;
V_s_p_sigma_5 = V_s_p_sigma_4 * decay_r_2;
V_p_p_sigma_5 = V_p_p_sigma_4 * decay_r_2;
V_p_p_pi_5 =    V_p_p_pi_4 * decay_r_2;

V_s_s_sigma_6 = V_s_s_sigma_4 * decay_r_2;
V_s_p_sigma_6 = V_s_p_sigma_4 * decay_r_2;
V_p_p_sigma_6 = V_p_p_sigma_4 * decay_r_2;
V_p_p_pi_6 =    V_p_p_pi_4 * decay_r_2;

V_s_s_sigma_7 = V_s_s_sigma_4 * decay_r_2;
V_s_p_sigma_7 = V_s_p_sigma_4 * decay_r_2;
V_p_p_sigma_7 = V_p_p_sigma_4 * decay_r_2;
V_p_p_pi_7 =    V_p_p_pi_4 * decay_r_2;

V_s_s_sigma_8 = V_s_s_sigma_4 * decay_r_2;
V_s_p_sigma_8 = V_s_p_sigma_4 * decay_r_2;
V_p_p_sigma_8 = V_p_p_sigma_4 * decay_r_2;
V_p_p_pi_8 =    V_p_p_pi_4 * decay_r_2;

V_s_s_sigma_9 = V_s_s_sigma_4 * decay_r_2;
V_s_p_sigma_9 = V_s_p_sigma_4 * decay_r_2;
V_p_p_sigma_9 = V_p_p_sigma_4 * decay_r_2;
V_p_p_pi_9 =    V_p_p_pi_4 * decay_r_2;
%---------------------------------------------------------------%

decay_r_3 = exp((distance_1 - distance_3)/((a - distance_1)/(log(10))));

V_s_s_sigma_10 = -1.0 * decay_r_3;
V_s_p_sigma_10 = -2.90 * decay_r_3;
V_p_p_sigma_10 = 3.30 * decay_r_3;
V_p_p_pi_10 = -0.70 * decay_r_3;

V_s_s_sigma_11 = -1.0 * decay_r_3;
V_s_p_sigma_11 = -2.90 * decay_r_3;
V_p_p_sigma_11 = 3.30 * decay_r_3;
V_p_p_pi_11 = -0.70 * decay_r_3;

V_s_s_sigma_12 = -1.0 * decay_r_3;
V_s_p_sigma_12 = -2.90 * decay_r_3;
V_p_p_sigma_12 = 3.30 * decay_r_3;
V_p_p_pi_12 = -0.70 * decay_r_3;
%---------------------------------------------------------------%

decay_r_4 = exp((distance_1 - distance_4)/((a - distance_1)/(log(10))));

V_s_s_sigma_13 = -1.0 * decay_r_4;
V_s_p_sigma_13 = -2.90 * decay_r_4;
V_p_p_sigma_13 = 3.30 * decay_r_4;
V_p_p_pi_13 = -0.70 * decay_r_4;

V_s_s_sigma_14 = -1.0 * decay_r_4;
V_s_p_sigma_14 = -2.90 * decay_r_4;
V_p_p_sigma_14 = 3.30 * decay_r_4;
V_p_p_pi_14 = -0.70 * decay_r_4;

V_s_s_sigma_15 = -1.0 * decay_r_4;
V_s_p_sigma_15 = -2.90 * decay_r_4;
V_p_p_sigma_15 = 3.30 * decay_r_4;
V_p_p_pi_15 = -0.70 * decay_r_4;

V_s_s_sigma_16 = -1.0 * decay_r_4;
V_s_p_sigma_16 = -2.90 * decay_r_4;
V_p_p_sigma_16 = 3.30 * decay_r_4;
V_p_p_pi_16 = -0.70 * decay_r_4;

V_s_s_sigma_17 = -1.0 * decay_r_4;
V_s_p_sigma_17 = -2.90 * decay_r_4;
V_p_p_sigma_17 = 3.30 * decay_r_4;
V_p_p_pi_17 = -0.70 * decay_r_4;

V_s_s_sigma_18 = -1.0 * decay_r_4;
V_s_p_sigma_18 = -2.90 * decay_r_4;
V_p_p_sigma_18 = 3.30 * decay_r_4;
V_p_p_pi_18 = -0.70 * decay_r_4;
%---------------------------------------------------------------%

decay_r_5 = exp((distance_1 - distance_5)/((a - distance_1)/(log(10))));

V_s_s_sigma_19 = -1.0 * decay_r_5;
V_s_p_sigma_19 = -2.90 * decay_r_5;
V_p_p_sigma_19 = 3.30 * decay_r_5;
V_p_p_pi_19 = -0.70 * decay_r_5;

V_s_s_sigma_20 = -1.0 * decay_r_5;
V_s_p_sigma_20 = -2.90 * decay_r_5;
V_p_p_sigma_20 = 3.30 * decay_r_5;
V_p_p_pi_20 = -0.70 * decay_r_5;

V_s_s_sigma_21 = -1.0 * decay_r_5;
V_s_p_sigma_21 = -2.90 * decay_r_5;
V_p_p_sigma_21 = 3.30 * decay_r_5;
V_p_p_pi_21 = -0.70 * decay_r_5;

V_s_s_sigma_22 = -1.0 * decay_r_5;
V_s_p_sigma_22 = -2.90 * decay_r_5;
V_p_p_sigma_22 = 3.30 * decay_r_5;
V_p_p_pi_22 = -0.70 * decay_r_5;

V_s_s_sigma_23 = -1.0 * decay_r_5;
V_s_p_sigma_23 = -2.90 * decay_r_5;
V_p_p_sigma_23 = 3.30 * decay_r_5;
V_p_p_pi_23 = -0.70 * decay_r_5;

V_s_s_sigma_24 = -1.0 * decay_r_5;
V_s_p_sigma_24 = -2.90 * decay_r_5;
V_p_p_sigma_24 = 3.30 * decay_r_5;
V_p_p_pi_24 = -0.70 * decay_r_5;
%---------------------------------------------------------------%

E_s_s_1 = V_s_s_sigma_1;
E_s_x_1 = (x_d_1/distance_1) * V_s_p_sigma_1;
E_s_y_1 = (y_d_1/distance_1) * V_s_p_sigma_1;
E_s_z_1 = (z_d_1/distance_1) * V_s_p_sigma_1;
E_x_y_1 = ((x_d_1 * y_d_1/(distance_1)^2)) * (V_p_p_sigma_1 - V_p_p_pi_1);
E_x_z_1 = ((x_d_1 * z_d_1/(distance_1)^2)) * (V_p_p_sigma_1 - V_p_p_pi_1);
E_y_z_1 = ((y_d_1 * z_d_1/(distance_1)^2)) * (V_p_p_sigma_1 - V_p_p_pi_1);
E_x_x_1 = ((x_d_1^2/(distance_1)^2) * V_p_p_sigma_1) + ((1 - (x_d_1^2/(distance_1)^2)) * V_p_p_pi_1);
E_y_y_1 = ((y_d_1^2/(distance_1)^2) * V_p_p_sigma_1) + ((1 - (y_d_1^2/(distance_1)^2)) * V_p_p_pi_1);
E_z_z_1 = ((z_d_1^2/(distance_1)^2) * V_p_p_sigma_1) + ((1 - (z_d_1^2/(distance_1)^2)) * V_p_p_pi_1);

E_s_s_2 = V_s_s_sigma_2;
E_s_x_2 = (x_d_2/distance_1) * V_s_p_sigma_2;
E_s_y_2 = (y_d_2/distance_1) * V_s_p_sigma_2;
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E_s_z_2 = (z_d_2/distance_1) * V_s_p_sigma_2;
E_x_y_2 = ((x_d_2 * y_d_2/(distance_1)^2)) * (V_p_p_sigma_2 - V_p_p_pi_2);
E_x_z_2 = ((x_d_2 * z_d_2/(distance_1)^2)) * (V_p_p_sigma_2 - V_p_p_pi_2);
E_y_z_2 = ((y_d_2 * z_d_2/(distance_1)^2)) * (V_p_p_sigma_2 - V_p_p_pi_2);
E_x_x_2 = ((x_d_2^2/(distance_1)^2) * V_p_p_sigma_2) + ((1 - (x_d_2^2/(distance_1)^2)) * V_p_p_pi_2);
E_y_y_2 = ((y_d_2^2/(distance_1)^2) * V_p_p_sigma_2) + ((1 - (y_d_2^2/(distance_1)^2)) * V_p_p_pi_2);
E_z_z_2 = ((z_d_2^2/(distance_1)^2) * V_p_p_sigma_2) + ((1 - (z_d_2^2/(distance_1)^2)) * V_p_p_pi_2);

E_s_s_3 = V_s_s_sigma_3;
E_s_x_3 = (x_d_3/distance_1) * V_s_p_sigma_3;
E_s_y_3 = (y_d_3/distance_1) * V_s_p_sigma_3;
E_s_z_3 = (z_d_3/distance_1) * V_s_p_sigma_3;
E_x_y_3 = ((x_d_3 * y_d_3/(distance_1)^2)) * (V_p_p_sigma_3 - V_p_p_pi_3);
E_x_z_3 = ((x_d_3 * z_d_3/(distance_1)^2)) * (V_p_p_sigma_3 - V_p_p_pi_3);
E_y_z_3 = ((y_d_3 * z_d_3/(distance_1)^2)) * (V_p_p_sigma_3 - V_p_p_pi_3);
E_x_x_3 = ((x_d_3^2/(distance_1)^2) * V_p_p_sigma_3) + ((1 - (x_d_3^2/(distance_1)^2)) * V_p_p_pi_3);
E_y_y_3 = ((y_d_3^2/(distance_1)^2) * V_p_p_sigma_3) + ((1 - (y_d_3^2/(distance_1)^2)) * V_p_p_pi_3);
E_z_z_3 = ((z_d_3^2/(distance_1)^2) * V_p_p_sigma_3) + ((1 - (z_d_3^2/(distance_1)^2)) * V_p_p_pi_3);
%--------------------------------------------------------------%

E_s_s_4 = V_s_s_sigma_4;
E_s_x_4 = (x_d_4/distance_2) * V_s_p_sigma_4;
E_s_y_4 = (y_d_4/distance_2) * V_s_p_sigma_4;
E_s_z_4 = (z_d_4/distance_2) * V_s_p_sigma_4;
E_x_y_4 = ((x_d_4 * y_d_4/(distance_2)^2)) * (V_p_p_sigma_4 - V_p_p_pi_4);
E_x_z_4 = ((x_d_4 * z_d_4/(distance_2)^2)) * (V_p_p_sigma_4 - V_p_p_pi_4);
E_y_z_4 = ((y_d_4 * z_d_4/(distance_2)^2)) * (V_p_p_sigma_4 - V_p_p_pi_4);
E_x_x_4 = ((x_d_4^2/(distance_2)^2) * V_p_p_sigma_4) + ((1 - (x_d_4^2/(distance_2)^2)) * V_p_p_pi_4);
E_y_y_4 = ((y_d_4^2/(distance_2)^2) * V_p_p_sigma_4) + ((1 - (y_d_4^2/(distance_2)^2)) * V_p_p_pi_4);
E_z_z_4 = ((z_d_4^2/(distance_2)^2) * V_p_p_sigma_4) + ((1 - (z_d_4^2/(distance_2)^2)) * V_p_p_pi_4);

E_s_s_5 = V_s_s_sigma_5;
E_s_x_5 = (x_d_5/distance_2) * V_s_p_sigma_5;
E_s_y_5 = (y_d_5/distance_2) * V_s_p_sigma_5;
E_s_z_5 = (z_d_5/distance_2) * V_s_p_sigma_5;
E_x_y_5 = ((x_d_5 * y_d_5/(distance_2)^2)) * (V_p_p_sigma_5 - V_p_p_pi_5);
E_x_z_5 = ((x_d_5 * z_d_5/(distance_2)^2)) * (V_p_p_sigma_5 - V_p_p_pi_5);
E_y_z_5 = ((y_d_5 * z_d_5/(distance_2)^2)) * (V_p_p_sigma_5 - V_p_p_pi_5);
E_x_x_5 = ((x_d_5^2/(distance_2)^2) * V_p_p_sigma_5) + ((1 - (x_d_5^2/(distance_2)^2)) * V_p_p_pi_5);
E_y_y_5 = ((y_d_5^2/(distance_2)^2) * V_p_p_sigma_5) + ((1 - (y_d_5^2/(distance_2)^2)) * V_p_p_pi_5);
E_z_z_5 = ((z_d_5^2/(distance_2)^2) * V_p_p_sigma_5) + ((1 - (z_d_5^2/(distance_2)^2)) * V_p_p_pi_5);

E_s_s_6 = V_s_s_sigma_6;
E_s_x_6 = (x_d_6/distance_2) * V_s_p_sigma_6;
E_s_y_6 = (y_d_6/distance_2) * V_s_p_sigma_6;
E_s_z_6 = (z_d_6/distance_2) * V_s_p_sigma_6;
E_x_y_6 = ((x_d_6 * y_d_6/(distance_2)^2)) * (V_p_p_sigma_6 - V_p_p_pi_6);
E_x_z_6 = ((x_d_6 * z_d_6/(distance_2)^2)) * (V_p_p_sigma_6 - V_p_p_pi_6);
E_y_z_6 = ((y_d_6 * z_d_6/(distance_2)^2)) * (V_p_p_sigma_6 - V_p_p_pi_6);
E_x_x_6 = ((x_d_6^2/(distance_2)^2) * V_p_p_sigma_6) + ((1 - (x_d_6^2/(distance_2)^2)) * V_p_p_pi_6);
E_y_y_6 = ((y_d_6^2/(distance_2)^2) * V_p_p_sigma_6) + ((1 - (y_d_6^2/(distance_2)^2)) * V_p_p_pi_6);
E_z_z_6 = ((z_d_6^2/(distance_2)^2) * V_p_p_sigma_6) + ((1 - (z_d_6^2/(distance_2)^2)) * V_p_p_pi_6);

E_s_s_7 = V_s_s_sigma_7;
E_s_x_7 = (x_d_7/distance_2) * V_s_p_sigma_7;
E_s_y_7 = (y_d_7/distance_2) * V_s_p_sigma_7;
E_s_z_7 = (z_d_7/distance_2) * V_s_p_sigma_7;
E_x_y_7 = ((x_d_7 * y_d_7/(distance_2)^2)) * (V_p_p_sigma_7 - V_p_p_pi_7);
E_x_z_7 = ((x_d_7 * z_d_7/(distance_2)^2)) * (V_p_p_sigma_7 - V_p_p_pi_7);
E_y_z_7 = ((y_d_7 * z_d_7/(distance_2)^2)) * (V_p_p_sigma_7 - V_p_p_pi_7);
E_x_x_7 = ((x_d_7^2/(distance_2)^2) * V_p_p_sigma_7) + ((1 - (x_d_7^2/(distance_2)^2)) * V_p_p_pi_7);
E_y_y_7 = ((y_d_7^2/(distance_2)^2) * V_p_p_sigma_7) + ((1 - (y_d_7^2/(distance_2)^2)) * V_p_p_pi_7);
E_z_z_7 = ((z_d_7^2/(distance_2)^2) * V_p_p_sigma_7) + ((1 - (z_d_7^2/(distance_2)^2)) * V_p_p_pi_7);

E_s_s_8 = V_s_s_sigma_8;
E_s_x_8 = (x_d_8/distance_2) * V_s_p_sigma_8;
E_s_y_8 = (y_d_8/distance_2) * V_s_p_sigma_8;
E_s_z_8 = (z_d_8/distance_2) * V_s_p_sigma_8;
E_x_y_8 = ((x_d_8 * y_d_8/(distance_2)^2)) * (V_p_p_sigma_8 - V_p_p_pi_8);
E_x_z_8 = ((x_d_8 * z_d_8/(distance_2)^2)) * (V_p_p_sigma_8 - V_p_p_pi_8);
E_y_z_8 = ((y_d_8 * z_d_8/(distance_2)^2)) * (V_p_p_sigma_8 - V_p_p_pi_8);
E_x_x_8 = ((x_d_8^2/(distance_2)^2) * V_p_p_sigma_8) + ((1 - (x_d_8^2/(distance_2)^2)) * V_p_p_pi_8);
E_y_y_8 = ((y_d_8^2/(distance_2)^2) * V_p_p_sigma_8) + ((1 - (y_d_8^2/(distance_2)^2)) * V_p_p_pi_8);
E_z_z_8 = ((z_d_8^2/(distance_2)^2) * V_p_p_sigma_8) + ((1 - (z_d_8^2/(distance_2)^2)) * V_p_p_pi_8);

E_s_s_9 = V_s_s_sigma_9;
E_s_x_9 = (x_d_9/distance_2) * V_s_p_sigma_9;
E_s_y_9 = (y_d_9/distance_2) * V_s_p_sigma_9;
E_s_z_9 = (z_d_9/distance_2) * V_s_p_sigma_9;
E_x_y_9 = ((x_d_9 * y_d_9/(distance_2)^2)) * (V_p_p_sigma_9 - V_p_p_pi_9);
E_x_z_9 = ((x_d_9 * z_d_9/(distance_2)^2)) * (V_p_p_sigma_9 - V_p_p_pi_9);
E_y_z_9 = ((y_d_9 * z_d_9/(distance_2)^2)) * (V_p_p_sigma_9 - V_p_p_pi_9);
E_x_x_9 = ((x_d_9^2/(distance_2)^2) * V_p_p_sigma_9) + ((1 - (x_d_9^2/(distance_2)^2)) * V_p_p_pi_9);
E_y_y_9 = ((y_d_9^2/(distance_2)^2) * V_p_p_sigma_9) + ((1 - (y_d_9^2/(distance_2)^2)) * V_p_p_pi_9);
E_z_z_9 = ((z_d_9^2/(distance_2)^2) * V_p_p_sigma_9) + ((1 - (z_d_9^2/(distance_2)^2)) * V_p_p_pi_9);
%--------------------------------------------------------------%

E_s_s_10 = V_s_s_sigma_10;
E_s_x_10 = (x_d_10/distance_3) * V_s_p_sigma_10;
E_s_y_10 = (y_d_10/distance_3) * V_s_p_sigma_10;
E_s_z_10 = (z_d_10/distance_3) * V_s_p_sigma_10;
E_x_y_10 = ((x_d_10 * y_d_10/(distance_3)^2)) * (V_p_p_sigma_10 - V_p_p_pi_10);
E_x_z_10 = ((x_d_10 * z_d_10/(distance_3)^2)) * (V_p_p_sigma_10 - V_p_p_pi_10);
E_y_z_10 = ((y_d_10 * z_d_10/(distance_3)^2)) * (V_p_p_sigma_10 - V_p_p_pi_10);
E_x_x_10 = ((x_d_10^2/(distance_3)^2) * V_p_p_sigma_10) + ((1 - (x_d_10^2/(distance_3)^2)) * V_p_p_pi_10);
E_y_y_10 = ((y_d_10^2/(distance_3)^2) * V_p_p_sigma_10) + ((1 - (y_d_10^2/(distance_3)^2)) * V_p_p_pi_10);
E_z_z_10 = ((z_d_10^2/(distance_3)^2) * V_p_p_sigma_10) + ((1 - (z_d_10^2/(distance_3)^2)) * V_p_p_pi_10);

E_s_s_11 = V_s_s_sigma_11;
E_s_x_11 = (x_d_11/distance_3) * V_s_p_sigma_11;
E_s_y_11 = (y_d_11/distance_3) * V_s_p_sigma_11;
E_s_z_11 = (z_d_11/distance_3) * V_s_p_sigma_11;
E_x_y_11 = ((x_d_11 * y_d_11/(distance_3)^2)) * (V_p_p_sigma_11 - V_p_p_pi_11);
E_x_z_11 = ((x_d_11 * z_d_11/(distance_3)^2)) * (V_p_p_sigma_11 - V_p_p_pi_11);
E_y_z_11 = ((y_d_11 * z_d_11/(distance_3)^2)) * (V_p_p_sigma_11 - V_p_p_pi_11);
E_x_x_11 = ((x_d_11^2/(distance_3)^2) * V_p_p_sigma_11) + ((1 - (x_d_11^2/(distance_3)^2)) * V_p_p_pi_11);
E_y_y_11 = ((y_d_11^2/(distance_3)^2) * V_p_p_sigma_11) + ((1 - (y_d_11^2/(distance_3)^2)) * V_p_p_pi_11);
E_z_z_11 = ((z_d_11^2/(distance_3)^2) * V_p_p_sigma_11) + ((1 - (z_d_11^2/(distance_3)^2)) * V_p_p_pi_11);

E_s_s_12 = V_s_s_sigma_12;
E_s_x_12 = (x_d_12/distance_3) * V_s_p_sigma_12;
E_s_y_12 = (y_d_12/distance_3) * V_s_p_sigma_12;
E_s_z_12 = (z_d_12/distance_3) * V_s_p_sigma_12;
E_x_y_12 = ((x_d_12 * y_d_12/(distance_3)^2)) * (V_p_p_sigma_12 - V_p_p_pi_12);
E_x_z_12 = ((x_d_12 * z_d_12/(distance_3)^2)) * (V_p_p_sigma_12 - V_p_p_pi_12);
E_y_z_12 = ((y_d_12 * z_d_12/(distance_3)^2)) * (V_p_p_sigma_12 - V_p_p_pi_12);
E_x_x_12 = ((x_d_12^2/(distance_3)^2) * V_p_p_sigma_12) + ((1 - (x_d_12^2/(distance_3)^2)) * V_p_p_pi_12);
E_y_y_12 = ((y_d_12^2/(distance_3)^2) * V_p_p_sigma_12) + ((1 - (y_d_12^2/(distance_3)^2)) * V_p_p_pi_12);
E_z_z_12 = ((z_d_12^2/(distance_3)^2) * V_p_p_sigma_12) + ((1 - (z_d_12^2/(distance_3)^2)) * V_p_p_pi_12);
%--------------------------------------------------------------%

E_s_s_13 = V_s_s_sigma_13;
E_s_x_13 = (x_d_13/distance_4) * V_s_p_sigma_13;
E_s_y_13 = (y_d_13/distance_4) * V_s_p_sigma_13;
E_s_z_13 = (z_d_13/distance_4) * V_s_p_sigma_13;
E_x_y_13 = ((x_d_13 * y_d_13/(distance_4)^2)) * (V_p_p_sigma_13 - V_p_p_pi_13);
E_x_z_13 = ((x_d_13 * z_d_13/(distance_4)^2)) * (V_p_p_sigma_13 - V_p_p_pi_13);
E_y_z_13 = ((y_d_13 * z_d_13/(distance_4)^2)) * (V_p_p_sigma_13 - V_p_p_pi_13);
E_x_x_13 = ((x_d_13^2/(distance_4)^2) * V_p_p_sigma_13) + ((1 - (x_d_13^2/(distance_4)^2)) * V_p_p_pi_13);
E_y_y_13 = ((y_d_13^2/(distance_4)^2) * V_p_p_sigma_13) + ((1 - (y_d_13^2/(distance_4)^2)) * V_p_p_pi_13);
E_z_z_13 = ((z_d_13^2/(distance_4)^2) * V_p_p_sigma_13) + ((1 - (z_d_13^2/(distance_4)^2)) * V_p_p_pi_13);

E_s_s_14 = V_s_s_sigma_14;
E_s_x_14 = (x_d_14/distance_4) * V_s_p_sigma_14;
E_s_y_14 = (y_d_14/distance_4) * V_s_p_sigma_14;
E_s_z_14 = (z_d_14/distance_4) * V_s_p_sigma_14;
E_x_y_14 = ((x_d_14 * y_d_14/(distance_4)^2)) * (V_p_p_sigma_14 - V_p_p_pi_14);
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E_x_z_14 = ((x_d_14 * z_d_14/(distance_4)^2)) * (V_p_p_sigma_14 - V_p_p_pi_14);
E_y_z_14 = ((y_d_14 * z_d_14/(distance_4)^2)) * (V_p_p_sigma_14 - V_p_p_pi_14);
E_x_x_14 = ((x_d_14^2/(distance_4)^2) * V_p_p_sigma_14) + ((1 - (x_d_14^2/(distance_4)^2)) * V_p_p_pi_14);
E_y_y_14 = ((y_d_14^2/(distance_4)^2) * V_p_p_sigma_14) + ((1 - (y_d_14^2/(distance_4)^2)) * V_p_p_pi_14);
E_z_z_14 = ((z_d_14^2/(distance_4)^2) * V_p_p_sigma_14) + ((1 - (z_d_14^2/(distance_4)^2)) * V_p_p_pi_14);

E_s_s_15 = V_s_s_sigma_15;
E_s_x_15 = (x_d_15/distance_4) * V_s_p_sigma_15;
E_s_y_15 = (y_d_15/distance_4) * V_s_p_sigma_15;
E_s_z_15 = (z_d_15/distance_4) * V_s_p_sigma_15;
E_x_y_15 = ((x_d_15 * y_d_15/(distance_4)^2)) * (V_p_p_sigma_15 - V_p_p_pi_15);
E_x_z_15 = ((x_d_15 * z_d_15/(distance_4)^2)) * (V_p_p_sigma_15 - V_p_p_pi_15);
E_y_z_15 = ((y_d_15 * z_d_15/(distance_4)^2)) * (V_p_p_sigma_15 - V_p_p_pi_15);
E_x_x_15 = ((x_d_15^2/(distance_4)^2) * V_p_p_sigma_15) + ((1 - (x_d_15^2/(distance_4)^2)) * V_p_p_pi_15);
E_y_y_15 = ((y_d_15^2/(distance_4)^2) * V_p_p_sigma_15) + ((1 - (y_d_15^2/(distance_4)^2)) * V_p_p_pi_15);
E_z_z_15 = ((z_d_15^2/(distance_4)^2) * V_p_p_sigma_15) + ((1 - (z_d_15^2/(distance_4)^2)) * V_p_p_pi_15);

E_s_s_16 = V_s_s_sigma_16;
E_s_x_16 = (x_d_16/distance_4) * V_s_p_sigma_16;
E_s_y_16 = (y_d_16/distance_4) * V_s_p_sigma_16;
E_s_z_16 = (z_d_16/distance_4) * V_s_p_sigma_16;
E_x_y_16 = ((x_d_16 * y_d_16/(distance_4)^2)) * (V_p_p_sigma_16 - V_p_p_pi_16);
E_x_z_16 = ((x_d_16 * z_d_16/(distance_4)^2)) * (V_p_p_sigma_16 - V_p_p_pi_16);
E_y_z_16 = ((y_d_16 * z_d_16/(distance_4)^2)) * (V_p_p_sigma_16 - V_p_p_pi_16);
E_x_x_16 = ((x_d_16^2/(distance_4)^2) * V_p_p_sigma_16) + ((1 - (x_d_16^2/(distance_4)^2)) * V_p_p_pi_16);
E_y_y_16 = ((y_d_16^2/(distance_4)^2) * V_p_p_sigma_16) + ((1 - (y_d_16^2/(distance_4)^2)) * V_p_p_pi_16);
E_z_z_16 = ((z_d_16^2/(distance_4)^2) * V_p_p_sigma_16) + ((1 - (z_d_16^2/(distance_4)^2)) * V_p_p_pi_16);

E_s_s_17 = V_s_s_sigma_17;
E_s_x_17 = (x_d_17/distance_4) * V_s_p_sigma_17;
E_s_y_17 = (y_d_17/distance_4) * V_s_p_sigma_17;
E_s_z_17 = (z_d_17/distance_4) * V_s_p_sigma_17;
E_x_y_17 = ((x_d_17 * y_d_17/(distance_4)^2)) * (V_p_p_sigma_17 - V_p_p_pi_17);
E_x_z_17 = ((x_d_17 * z_d_17/(distance_4)^2)) * (V_p_p_sigma_17 - V_p_p_pi_17);
E_y_z_17 = ((y_d_17 * z_d_17/(distance_4)^2)) * (V_p_p_sigma_17 - V_p_p_pi_17);
E_x_x_17 = ((x_d_17^2/(distance_4)^2) * V_p_p_sigma_17) + ((1 - (x_d_17^2/(distance_4)^2)) * V_p_p_pi_17);
E_y_y_17 = ((y_d_17^2/(distance_4)^2) * V_p_p_sigma_17) + ((1 - (y_d_17^2/(distance_4)^2)) * V_p_p_pi_17);
E_z_z_17 = ((z_d_17^2/(distance_4)^2) * V_p_p_sigma_17) + ((1 - (z_d_17^2/(distance_4)^2)) * V_p_p_pi_17);

E_s_s_18 = V_s_s_sigma_18;
E_s_x_18 = (x_d_18/distance_4) * V_s_p_sigma_18;
E_s_y_18 = (y_d_18/distance_4) * V_s_p_sigma_18;
E_s_z_18 = (z_d_18/distance_4) * V_s_p_sigma_18;
E_x_y_18 = ((x_d_18 * y_d_18/(distance_4)^2)) * (V_p_p_sigma_18 - V_p_p_pi_18);
E_x_z_18 = ((x_d_18 * z_d_18/(distance_4)^2)) * (V_p_p_sigma_18 - V_p_p_pi_18);
E_y_z_18 = ((y_d_18 * z_d_18/(distance_4)^2)) * (V_p_p_sigma_18 - V_p_p_pi_18);
E_x_x_18 = ((x_d_18^2/(distance_4)^2) * V_p_p_sigma_18) + ((1 - (x_d_18^2/(distance_4)^2)) * V_p_p_pi_18);
E_y_y_18 = ((y_d_18^2/(distance_4)^2) * V_p_p_sigma_18) + ((1 - (y_d_18^2/(distance_4)^2)) * V_p_p_pi_18);
E_z_z_18 = ((z_d_18^2/(distance_4)^2) * V_p_p_sigma_18) + ((1 - (z_d_18^2/(distance_4)^2)) * V_p_p_pi_18);
%---------------------------------------------------------------%

E_s_s_19 = V_s_s_sigma_19;
E_s_x_19 = (x_d_19/distance_5) * V_s_p_sigma_19;
E_s_y_19 = (y_d_19/distance_5) * V_s_p_sigma_19;
E_s_z_19 = (z_d_19/distance_5) * V_s_p_sigma_19;
E_x_y_19 = ((x_d_19 * y_d_19/(distance_5)^2)) * (V_p_p_sigma_19 - V_p_p_pi_19);
E_x_z_19 = ((x_d_19 * z_d_19/(distance_5)^2)) * (V_p_p_sigma_19 - V_p_p_pi_19);
E_y_z_19 = ((y_d_19 * z_d_19/(distance_5)^2)) * (V_p_p_sigma_19 - V_p_p_pi_19);
E_x_x_19 = ((x_d_19^2/(distance_5)^2) * V_p_p_sigma_19) + ((1 - (x_d_19^2/(distance_5)^2)) * V_p_p_pi_19);
E_y_y_19 = ((y_d_19^2/(distance_5)^2) * V_p_p_sigma_19) + ((1 - (y_d_19^2/(distance_5)^2)) * V_p_p_pi_19);
E_z_z_19 = ((z_d_19^2/(distance_5)^2) * V_p_p_sigma_19) + ((1 - (z_d_19^2/(distance_5)^2)) * V_p_p_pi_19);

E_s_s_20 = V_s_s_sigma_20;
E_s_x_20 = (x_d_20/distance_5) * V_s_p_sigma_20;
E_s_y_20 = (y_d_20/distance_5) * V_s_p_sigma_20;
E_s_z_20 = (z_d_20/distance_5) * V_s_p_sigma_20;
E_x_y_20 = ((x_d_20 * y_d_20/(distance_5)^2)) * (V_p_p_sigma_20 - V_p_p_pi_20);
E_x_z_20 = ((x_d_20 * z_d_20/(distance_5)^2)) * (V_p_p_sigma_20 - V_p_p_pi_20);
E_y_z_20 = ((y_d_20 * z_d_20/(distance_5)^2)) * (V_p_p_sigma_20 - V_p_p_pi_20);
E_x_x_20 = ((x_d_20^2/(distance_5)^2) * V_p_p_sigma_20) + ((1 - (x_d_20^2/(distance_5)^2)) * V_p_p_pi_20);
E_y_y_20 = ((y_d_20^2/(distance_5)^2) * V_p_p_sigma_20) + ((1 - (y_d_20^2/(distance_5)^2)) * V_p_p_pi_20);
E_z_z_20 = ((z_d_20^2/(distance_5)^2) * V_p_p_sigma_20) + ((1 - (z_d_20^2/(distance_5)^2)) * V_p_p_pi_20);

E_s_s_21 = V_s_s_sigma_21;
E_s_x_21 = (x_d_21/distance_5) * V_s_p_sigma_21;
E_s_y_21 = (y_d_21/distance_5) * V_s_p_sigma_21;
E_s_z_21 = (z_d_21/distance_5) * V_s_p_sigma_21;
E_x_y_21 = ((x_d_21 * y_d_21/(distance_5)^2)) * (V_p_p_sigma_21 - V_p_p_pi_21);
E_x_z_21 = ((x_d_21 * z_d_21/(distance_5)^2)) * (V_p_p_sigma_21 - V_p_p_pi_21);
E_y_z_21 = ((y_d_21 * z_d_21/(distance_5)^2)) * (V_p_p_sigma_21 - V_p_p_pi_21);
E_x_x_21 = ((x_d_21^2/(distance_5)^2) * V_p_p_sigma_21) + ((1 - (x_d_21^2/(distance_5)^2)) * V_p_p_pi_21);
E_y_y_21 = ((y_d_21^2/(distance_5)^2) * V_p_p_sigma_21) + ((1 - (y_d_21^2/(distance_5)^2)) * V_p_p_pi_21);
E_z_z_21 = ((z_d_21^2/(distance_5)^2) * V_p_p_sigma_21) + ((1 - (z_d_21^2/(distance_5)^2)) * V_p_p_pi_21);

E_s_s_22 = V_s_s_sigma_22;
E_s_x_22 = (x_d_22/distance_5) * V_s_p_sigma_22;
E_s_y_22 = (y_d_22/distance_5) * V_s_p_sigma_22;
E_s_z_22 = (z_d_22/distance_5) * V_s_p_sigma_22;
E_x_y_22 = ((x_d_22 * y_d_22/(distance_5)^2)) * (V_p_p_sigma_22 - V_p_p_pi_22);
E_x_z_22 = ((x_d_22 * z_d_22/(distance_5)^2)) * (V_p_p_sigma_22 - V_p_p_pi_22);
E_y_z_22 = ((y_d_22 * z_d_22/(distance_5)^2)) * (V_p_p_sigma_22 - V_p_p_pi_22);
E_x_x_22 = ((x_d_22^2/(distance_5)^2) * V_p_p_sigma_22) + ((1 - (x_d_22^2/(distance_5)^2)) * V_p_p_pi_22);
E_y_y_22 = ((y_d_22^2/(distance_5)^2) * V_p_p_sigma_22) + ((1 - (y_d_22^2/(distance_5)^2)) * V_p_p_pi_22);
E_z_z_22 = ((z_d_22^2/(distance_5)^2) * V_p_p_sigma_22) + ((1 - (z_d_22^2/(distance_5)^2)) * V_p_p_pi_22);

E_s_s_23 = V_s_s_sigma_23;
E_s_x_23 = (x_d_23/distance_5) * V_s_p_sigma_23;
E_s_y_23 = (y_d_23/distance_5) * V_s_p_sigma_23;
E_s_z_23 = (z_d_23/distance_5) * V_s_p_sigma_23;
E_x_y_23 = ((x_d_23 * y_d_23/(distance_5)^2)) * (V_p_p_sigma_23 - V_p_p_pi_23);
E_x_z_23 = ((x_d_23 * z_d_23/(distance_5)^2)) * (V_p_p_sigma_23 - V_p_p_pi_23);
E_y_z_23 = ((y_d_23 * z_d_23/(distance_5)^2)) * (V_p_p_sigma_23 - V_p_p_pi_23);
E_x_x_23 = ((x_d_23^2/(distance_5)^2) * V_p_p_sigma_23) + ((1 - (x_d_23^2/(distance_5)^2)) * V_p_p_pi_23);
E_y_y_23 = ((y_d_23^2/(distance_5)^2) * V_p_p_sigma_23) + ((1 - (y_d_23^2/(distance_5)^2)) * V_p_p_pi_23);
E_z_z_23 = ((z_d_23^2/(distance_5)^2) * V_p_p_sigma_23) + ((1 - (z_d_23^2/(distance_5)^2)) * V_p_p_pi_23);

E_s_s_24 = V_s_s_sigma_24;
E_s_x_24 = (x_d_24/distance_5) * V_s_p_sigma_24;
E_s_y_24 = (y_d_24/distance_5) * V_s_p_sigma_24;
E_s_z_24 = (z_d_24/distance_5) * V_s_p_sigma_24;
E_x_y_24 = ((x_d_24 * y_d_24/(distance_5)^2)) * (V_p_p_sigma_24 - V_p_p_pi_24);
E_x_z_24 = ((x_d_24 * z_d_24/(distance_5)^2)) * (V_p_p_sigma_24 - V_p_p_pi_24);
E_y_z_24 = ((y_d_24 * z_d_24/(distance_5)^2)) * (V_p_p_sigma_24 - V_p_p_pi_24);
E_x_x_24 = ((x_d_24^2/(distance_5)^2) * V_p_p_sigma_24) + ((1 - (x_d_24^2/(distance_5)^2)) * V_p_p_pi_24);
E_y_y_24 = ((y_d_24^2/(distance_5)^2) * V_p_p_sigma_24) + ((1 - (y_d_24^2/(distance_5)^2)) * V_p_p_pi_24);
E_z_z_24 = ((z_d_24^2/(distance_5)^2) * V_p_p_sigma_24) + ((1 - (z_d_24^2/(distance_5)^2)) * V_p_p_pi_24);
%---------------------------------------------------------------%

%---------------------------------------------------------------%
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%-------------------Gamma-M direction---------------------------%
k_x_1 = 0; k_y = (2 * pi)/sqrt(3)/a; k_z = 0; kmax = 1; Nt = 101;
for Nk = 1:Nt
   k = [k_x_1 k_y k_z] * kmax * (Nk - 1) / (Nt - 1);
%---------------------------------------------------------------%

%-------------Phase factors-------------------------------------%
   g_1_plus = exp(1i*sum(k.*d_1));
   g_2_plus = exp(1i*sum(k.*d_2));
   g_3_plus = exp(1i*sum(k.*d_3));
%---------------------------------------------------------------%
   g_4_plus = exp(1i*sum(k.*d_4));
   g_5_plus = exp(1i*sum(k.*d_5));
   g_6_plus = exp(1i*sum(k.*d_6));
   g_7_plus = exp(1i*sum(k.*d_7));
   g_8_plus = exp(1i*sum(k.*d_8));
   g_9_plus = exp(1i*sum(k.*d_9));
%---------------------------------------------------------------%
   g_10_plus = exp(1i*sum(k.*d_10));
   g_11_plus = exp(1i*sum(k.*d_11));
   g_12_plus = exp(1i*sum(k.*d_12));
%---------------------------------------------------------------%
   g_13_plus = exp(1i*sum(k.*d_13));
   g_14_plus = exp(1i*sum(k.*d_14));
   g_15_plus = exp(1i*sum(k.*d_15));
   g_16_plus = exp(1i*sum(k.*d_16));
   g_17_plus = exp(1i*sum(k.*d_17));
   g_18_plus = exp(1i*sum(k.*d_18));
%---------------------------------------------------------------%
   g_19_plus = exp(1i*sum(k.*d_19));
   g_20_plus = exp(1i*sum(k.*d_20));
   g_21_plus = exp(1i*sum(k.*d_21));
   g_22_plus = exp(1i*sum(k.*d_22));
   g_23_plus = exp(1i*sum(k.*d_23));
   g_24_plus = exp(1i*sum(k.*d_24));
%---------------------------------------------------------------%
   g_k = g_1_plus + g_2_plus + g_3_plus;
   g_k_2_3_minus = g_3_plus - g_2_plus;
   g_k_2_3_plus =  g_3_plus + g_2_plus;
   g_k_3_2_minus = g_2_plus - g_3_plus;
%---------------------------------------------------------------%
   g_k_2 = g_4_plus + g_5_plus + g_6_plus + g_7_plus + g_8_plus + g_9_plus;
   g_k_4_9 =       g_4_plus - g_5_plus + g_8_plus - g_9_plus;
   g_k_6_7_minus =   g_6_plus - g_7_plus;
   g_k_6_7_plus =    g_6_plus + g_7_plus;
   g_k_4_9_minus =   g_4_plus + g_5_plus - g_8_plus - g_9_plus;
   g_k_4_9_plus =    g_4_plus + g_5_plus + g_8_plus + g_9_plus;
   g_k_4_9_minus_1 = g_4_plus - g_5_plus - g_8_plus + g_9_plus;
%---------------------------------------------------------------%
   g_k_3 = g_10_plus + g_11_plus + g_12_plus;
   g_k_10_11_minus = g_10_plus - g_11_plus;
   g_k_10_11_plus =  g_10_plus + g_11_plus;
%---------------------------------------------------------------%
   g_k_4 = g_13_plus + g_14_plus + g_15_plus + g_16_plus + g_17_plus +
g_18_plus;
   g_k_13_14_minus = g_13_plus - g_14_plus;
   g_k_15_16_minus = g_15_plus - g_16_plus;
   g_k_17_18_minus = g_17_plus - g_18_plus;
   g_k_13_14_plus =  g_13_plus + g_14_plus;
   g_k_15_16_plus =  g_15_plus + g_16_plus;
   g_k_16_15_minus = g_16_plus - g_15_plus;
   g_k_17_18_plus =  g_17_plus + g_18_plus;
   g_k_18_17_minus = g_18_plus - g_17_plus;
%---------------------------------------------------------------%
   g_k_5 = g_19_plus + g_20_plus + g_21_plus + g_22_plus + g_23_plus +
g_24_plus;
   g_k_19_23_minus =   g_19_plus - g_23_plus;
   g_k_19_23_plus =    g_19_plus + g_23_plus;
   g_k_20_24 =       g_20_plus + g_22_plus - g_21_plus - g_24_plus;
   g_k_20_24_minus =   g_20_plus + g_21_plus - g_22_plus - g_24_plus;
   g_k_20_24_minus_1 = g_20_plus - g_21_plus - g_22_plus + g_24_plus;
   g_k_20_24_plus =    g_20_plus + g_21_plus + g_22_plus + g_24_plus;
%---------------------------------------------------------------%

%-------------Hamiltonian matrix--------------------------------%
   n = 0;
   Delta = n * eye(4);
%---------------------------------------------------------------%
   M_0 = [Epsilon_s 0 0 0
         0 Epsilon_p_x 0 0
         0 0 Epsilon_p_y 0
         0 0 0 Epsilon_p_z]; %On-sites energies of the 4 atomic sites
%---------------------------------------------------------------%
   M_0_apostrophe = [E_s_s_4*(g_k_2) E_s_x_4*(g_k_4_9) +
E_s_x_6*(g_k_6_7_minus) E_s_y_4*(g_k_4_9_minus) 0
              -E_s_x_4*(g_k_4_9) - E_s_x_6*(g_k_6_7_minus)
E_x_x_4*(g_k_4_9_plus) + E_x_x_6*(g_k_6_7_plus)
E_x_y_4*(g_k_4_9_minus_1) 0
              -E_s_y_4*(g_k_4_9_minus) E_x_y_4*(g_k_4_9_minus_1)
E_y_y_4*(g_k_4_9_plus) + E_y_y_6*(g_k_6_7_plus) 0
               0 0 0 E_z_z_9*(g_k_2)];
%---------------------------------------------------------------%
   M_0_apostrophe_1 = [E_s_s_19*(g_k_5) E_s_x_20*(g_k_20_24)
E_s_y_19*(g_k_19_23_minus) + E_s_y_20*(g_k_20_24_minus) 0
              -E_s_x_20*(g_k_20_24) E_x_x_19*(g_k_19_23_plus) +
E_x_x_20*(g_k_20_24_plus) E_x_y_20*(g_k_20_24_minus_1) 0
              -E_s_y_19*(g_k_19_23_minus) - E_s_y_20*(g_k_20_24_minus)
E_x_y_20*(g_k_20_24_minus_1) E_y_y_19*(g_k_19_23_plus) +
E_y_y_20*(g_k_20_24_plus) 0
               0 0 0 E_z_z_19*(g_k_5)];
%---------------------------------------------------------------%
   M_1 = [E_s_s_1*(g_k) E_s_x_3*(g_k_2_3_minus) E_s_y_1*(g_1_plus) +
E_s_y_3*(g_k_2_3_plus) E_s_z_3*(g_k)
       -E_s_x_3*(g_k_2_3_minus) E_x_x_1*(g_1_plus) +
E_x_x_3*(g_k_2_3_plus) E_x_y_2*(g_k_3_2_minus) E_x_z_3*(g_k_2_3_minus)
       -E_s_y_1*(g_1_plus) - E_s_y_3*(g_k_2_3_plus)
E_x_y_2*(g_k_3_2_minus) E_y_y_1*(g_1_plus) + E_y_y_3*(g_k_2_3_plus)
E_y_z_1*(g_1_plus) + E_y_z_3*(g_k_2_3_plus)
       -E_s_z_3*(g_k) E_x_z_3*(g_k_2_3_minus) E_y_z_1*(g_1_plus) +
E_y_z_3*(g_k_2_3_plus) E_z_z_1*(g_k)]; %NN coupling between A and B (B'
and A')
%---------------------------------------------------------------%
   M_1_apostrophe = [E_s_s_10*(g_k_3) E_s_x_10*(g_k_10_11_minus)
E_s_y_10*(g_k_10_11_plus) + E_s_y_12*(g_12_plus) E_s_z_10*(g_k_3)
             -E_s_x_10*(g_k_10_11_minus) E_x_x_10*(g_k_10_11_plus) +
E_x_x_12*(g_12_plus) E_x_y_10*(g_k_10_11_minus)
E_x_z_10*(g_k_10_11_minus)
             -E_s_y_10*(g_k_10_11_plus) - E_s_y_12*(g_12_plus)
E_x_y_10*(g_k_10_11_minus) E_y_y_10*(g_k_10_11_plus) +
E_y_y_12*(g_12_plus) E_y_z_10*(g_k_10_11_plus) + E_y_z_12*(g_12_plus)
             -E_s_z_10*(g_k_3) E_x_z_10*(g_k_10_11_minus)
E_y_z_10*(g_k_10_11_plus) + E_y_z_12*(g_12_plus) E_z_z_10*(g_k_3)];
%---------------------------------------------------------------%
   M_1_apostrophe_1 = [E_s_s_13*(g_k_4) E_s_x_13*(g_k_13_14_minus) +
E_s_x_15*(g_k_15_16_minus) + E_s_x_17*(g_k_17_18_minus)
E_s_y_13*(g_k_13_14_plus) + E_s_y_15*(g_k_15_16_plus) +
E_s_y_18*(g_k_17_18_plus) E_s_z_13*(g_k_4)
              -E_s_x_13*(g_k_13_14_minus) - E_s_x_15*(g_k_15_16_minus) -
E_s_x_17*(g_k_17_18_minus) E_x_x_13*(g_k_13_14_plus) +
E_x_x_15*(g_k_15_16_plus) + E_x_x_18*(g_k_17_18_plus)
E_x_y_13*(g_k_13_14_minus) + E_x_y_16*(g_k_16_15_minus) +
E_x_y_18*(g_k_18_17_minus) E_x_z_13*(g_k_13_14_minus) +
E_x_z_15*(g_k_15_16_minus) + E_x_z_17*(g_k_17_18_minus)
              -E_s_y_13*(g_k_13_14_plus) - E_s_y_15*(g_k_15_16_plus) -
E_s_y_18*(g_k_17_18_plus) E_x_y_13*(g_k_13_14_minus) +
E_x_y_16*(g_k_16_15_minus) + E_x_y_18*(g_k_18_17_minus)
E_y_y_13*(g_k_13_14_plus) + E_y_y_15*(g_k_15_16_plus) +
E_y_y_17*(g_k_17_18_plus) E_y_z_13*(g_k_13_14_plus) +
E_y_z_15*(g_k_15_16_plus) + E_y_z_17*(g_k_17_18_plus)
              -E_s_z_13*(g_k_4) E_x_z_13*(g_k_13_14_minus) +
E_x_z_15*(g_k_15_16_minus) + E_x_z_17*(g_k_17_18_minus)
E_y_z_13*(g_k_13_14_plus) + E_y_z_15*(g_k_15_16_plus) +
E_y_z_17*(g_k_17_18_plus) E_z_z_13*(g_k_4)];
%---------------------------------------------------------------%
   M_1_trans = M_1'; %NN coupling between A' and B'
   M_1_apostrophe_trans = M_1_apostrophe';
   M_1_apostrophe_1_trans = M_1_apostrophe_1';
%---------------------------------------------------------------%
   H = [M_0 + Delta + M_0_apostrophe + M_0_apostrophe_1 M_1 +
M_1_apostrophe + M_1_apostrophe_1
      M_1_trans + M_1_apostrophe_trans + M_1_apostrophe_1_trans M_0 -
Delta + M_0_apostrophe + M_0_apostrophe_1];
%---------------------------------------------------------------%
   [V,D] = eig(H);
   eigst = sum(D);
   E_1(Nk,:) = sort (real(eigst)); %#ok<*SAGROW>
%---------------------------------------------------------------%
end
figure;
hold on;
%---------------------------------------------------------------%
X_1 = linspace(150, 250, 101);
plot(X_1, E_1 + 3.8, 'k', 'LineWidth', 1.5);
%---------------------------------------------------------------%

%---------------------------------------------------------------%

%-------------------Gamma-K (-ve) direction---------------------%
k_x_2 = (2 * pi)/3/a; k_y = (2 * pi)/sqrt(3)/a; k_z = 0; kmax = 1; Nt = 101;
for Nk = 1:Nt
   k = [k_x_2 k_y k_z] * kmax * (Nk - 1)/(Nt - 1);
%---------------------------------------------------------------%

%-------------Phase factors-------------------------------------%
   g_1_plus = exp(1i*sum(k.*d_1));
   g_2_plus = exp(1i*sum(k.*d_2));
   g_3_plus = exp(1i*sum(k.*d_3));
%---------------------------------------------------------------%
   g_4_plus = exp(1i*sum(k.*d_4));
   g_5_plus = exp(1i*sum(k.*d_5));
   g_6_plus = exp(1i*sum(k.*d_6));
   g_7_plus = exp(1i*sum(k.*d_7));
   g_8_plus = exp(1i*sum(k.*d_8));
   g_9_plus = exp(1i*sum(k.*d_9));
%---------------------------------------------------------------%
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   g_10_plus = exp(1i*sum(k.*d_10));
   g_11_plus = exp(1i*sum(k.*d_11));
   g_12_plus = exp(1i*sum(k.*d_12));
%---------------------------------------------------------------%
   g_13_plus = exp(1i*sum(k.*d_13));
   g_14_plus = exp(1i*sum(k.*d_14));
   g_15_plus = exp(1i*sum(k.*d_15));
   g_16_plus = exp(1i*sum(k.*d_16));
   g_17_plus = exp(1i*sum(k.*d_17));
   g_18_plus = exp(1i*sum(k.*d_18));
%---------------------------------------------------------------%
   g_19_plus = exp(1i*sum(k.*d_19));
   g_20_plus = exp(1i*sum(k.*d_20));
   g_21_plus = exp(1i*sum(k.*d_21));
   g_22_plus = exp(1i*sum(k.*d_22));
   g_23_plus = exp(1i*sum(k.*d_23));
   g_24_plus = exp(1i*sum(k.*d_24));
%---------------------------------------------------------------%
   g_k = g_1_plus + g_2_plus + g_3_plus;
   g_k_2_3_minus = g_3_plus - g_2_plus;
   g_k_2_3_plus =  g_3_plus + g_2_plus;
   g_k_3_2_minus = g_2_plus - g_3_plus;
%---------------------------------------------------------------%
   g_k_2 = g_4_plus + g_5_plus + g_6_plus + g_7_plus + g_8_plus + g_9_plus;
   g_k_4_9 =        g_4_plus - g_5_plus + g_8_plus - g_9_plus;
   g_k_6_7_minus =   g_6_plus - g_7_plus;
   g_k_6_7_plus =    g_6_plus + g_7_plus;
   g_k_4_9_minus =   g_4_plus + g_5_plus - g_8_plus - g_9_plus;
   g_k_4_9_plus =    g_4_plus + g_5_plus + g_8_plus + g_9_plus;
   g_k_4_9_minus_1 = g_4_plus - g_5_plus - g_8_plus + g_9_plus;
%---------------------------------------------------------------%
   g_k_3 = g_10_plus + g_11_plus + g_12_plus;
   g_k_10_11_minus = g_10_plus - g_11_plus;
   g_k_10_11_plus =  g_10_plus + g_11_plus;
%---------------------------------------------------------------%
   g_k_4 = g_13_plus + g_14_plus + g_15_plus + g_16_plus + g_17_plus +
g_18_plus;
   g_k_13_14_minus = g_13_plus - g_14_plus;
   g_k_15_16_minus = g_15_plus - g_16_plus;
   g_k_17_18_minus = g_17_plus - g_18_plus;
   g_k_13_14_plus =  g_13_plus + g_14_plus;
   g_k_15_16_plus =  g_15_plus + g_16_plus;
   g_k_16_15_minus = g_16_plus - g_15_plus;
   g_k_17_18_plus =  g_17_plus + g_18_plus;
   g_k_18_17_minus = g_18_plus - g_17_plus;
%---------------------------------------------------------------%
   g_k_5 = g_19_plus + g_20_plus + g_21_plus + g_22_plus + g_23_plus +
g_24_plus;
   g_k_19_23_minus =   g_19_plus - g_23_plus;
   g_k_19_23_plus =    g_19_plus + g_23_plus;
   g_k_20_24 =        g_20_plus + g_22_plus - g_21_plus - g_24_plus;
   g_k_20_24_minus =   g_20_plus + g_21_plus - g_22_plus - g_24_plus;
   g_k_20_24_minus_1 = g_20_plus - g_21_plus - g_22_plus + g_24_plus;
   g_k_20_24_plus =    g_20_plus + g_21_plus + g_22_plus + g_24_plus;
%---------------------------------------------------------------%

%-------------Hamiltonian matrix--------------------------------%
   n = 0;
   Delta = n * eye(4);
%---------------------------------------------------------------%
   M_0 = [Epsilon_s 0 0 0
        0 Epsilon_p_x 0 0
        0 0 Epsilon_p_y 0
        0 0 0 Epsilon_p_z]; %On-sites energies of the 4 atomic sites
%---------------------------------------------------------------%
   M_0_apostrophe = [E_s_s_4*(g_k_2) E_s_x_4*(g_k_4_9) +
E_s_x_6*(g_k_6_7_minus) E_s_y_4*(g_k_4_9_minus) 0
             -E_s_x_4*(g_k_4_9) - E_s_x_6*(g_k_6_7_minus)
E_x_x_4*(g_k_4_9_plus) + E_x_x_6*(g_k_6_7_plus)
E_x_y_4*(g_k_4_9_minus_1) 0
             -E_s_y_4*(g_k_4_9_minus) E_x_y_4*(g_k_4_9_minus_1)
E_y_y_4*(g_k_4_9_plus) + E_y_y_6*(g_k_6_7_plus) 0
              0 0 0 E_z_z_9*(g_k_2)];
%---------------------------------------------------------------%
   M_0_apostrophe_1 = [E_s_s_19*(g_k_5) E_s_x_20*(g_k_20_24)
E_s_y_19*(g_k_19_23_minus) + E_s_y_20*(g_k_20_24_minus) 0
               -E_s_x_20*(g_k_20_24) E_x_x_19*(g_k_19_23_plus) +
E_x_x_20*(g_k_20_24_plus) E_x_y_20*(g_k_20_24_minus_1) 0
               -E_s_y_19*(g_k_19_23_minus) - E_s_y_20*(g_k_20_24_minus)
E_x_y_20*(g_k_20_24_minus_1) E_y_y_19*(g_k_19_23_plus) +
E_y_y_20*(g_k_20_24_plus) 0
               0 0 0 E_z_z_19*(g_k_5)];
%---------------------------------------------------------------%
   M_1 = [E_s_s_1*(g_k) E_s_x_3*(g_k_2_3_minus) E_s_y_1*(g_1_plus) +
E_s_y_3*(g_k_2_3_plus) E_s_z_3*(g_k)
       -E_s_x_3*(g_k_2_3_minus) E_x_x_1*(g_1_plus) +
E_x_x_3*(g_k_2_3_plus) E_x_y_2*(g_k_3_2_minus) E_x_z_3*(g_k_2_3_minus)
       -E_s_y_1*(g_1_plus) - E_s_y_3*(g_k_2_3_plus)
E_x_y_2*(g_k_3_2_minus) E_y_y_1*(g_1_plus) + E_y_y_3*(g_k_2_3_plus)
E_y_z_1*(g_1_plus) + E_y_z_3*(g_k_2_3_plus)
       -E_s_z_3*(g_k) E_x_z_3*(g_k_2_3_minus) E_y_z_1*(g_1_plus) +
E_y_z_3*(g_k_2_3_plus) E_z_z_1*(g_k)]; %NN coupling between A and B (B'
and A')
%---------------------------------------------------------------%
   M_1_apostrophe = [E_s_s_10*(g_k_3) E_s_x_10*(g_k_10_11_minus)
E_s_y_10*(g_k_10_11_plus) + E_s_y_12*(g_12_plus) E_s_z_10*(g_k_3)
             -E_s_x_10*(g_k_10_11_minus) E_x_x_10*(g_k_10_11_plus) +
E_x_x_12*(g_12_plus) E_x_y_10*(g_k_10_11_minus)
E_x_z_10*(g_k_10_11_minus)
             -E_s_y_10*(g_k_10_11_plus) - E_s_y_12*(g_12_plus)
E_x_y_10*(g_k_10_11_minus) E_y_y_10*(g_k_10_11_plus) +
E_y_y_12*(g_12_plus) E_y_z_10*(g_k_10_11_plus) + E_y_z_12*(g_12_plus)
             -E_s_z_10*(g_k_3) E_x_z_10*(g_k_10_11_minus)
E_y_z_10*(g_k_10_11_plus) + E_y_z_12*(g_12_plus) E_z_z_10*(g_k_3)];
%---------------------------------------------------------------%
   M_1_apostrophe_1 = [E_s_s_13*(g_k_4) E_s_x_13*(g_k_13_14_minus) +
E_s_x_15*(g_k_15_16_minus) + E_s_x_17*(g_k_17_18_minus)
E_s_y_13*(g_k_13_14_plus) + E_s_y_15*(g_k_15_16_plus) +
E_s_y_18*(g_k_17_18_plus) E_s_z_13*(g_k_4)
              -E_s_x_13*(g_k_13_14_minus) - E_s_x_15*(g_k_15_16_minus) -
E_s_x_17*(g_k_17_18_minus) E_x_x_13*(g_k_13_14_plus) +
E_x_x_15*(g_k_15_16_plus) + E_x_x_18*(g_k_17_18_plus)
E_x_y_13*(g_k_13_14_minus) + E_x_y_16*(g_k_16_15_minus) +
E_x_y_18*(g_k_18_17_minus) E_x_z_13*(g_k_13_14_minus) +
E_x_z_15*(g_k_15_16_minus) + E_x_z_17*(g_k_17_18_minus)
              -E_s_y_13*(g_k_13_14_plus) - E_s_y_15*(g_k_15_16_plus) -
E_s_y_18*(g_k_17_18_plus) E_x_y_13*(g_k_13_14_minus) +
E_x_y_16*(g_k_16_15_minus) + E_x_y_18*(g_k_18_17_minus)
E_y_y_13*(g_k_13_14_plus) + E_y_y_15*(g_k_15_16_plus) +
E_y_y_17*(g_k_17_18_plus) E_y_z_13*(g_k_13_14_plus) +
E_y_z_15*(g_k_15_16_plus) + E_y_z_17*(g_k_17_18_plus)
              -E_s_z_13*(g_k_4) E_x_z_13*(g_k_13_14_minus) +
E_x_z_15*(g_k_15_16_minus) + E_x_z_17*(g_k_17_18_minus)
E_y_z_13*(g_k_13_14_plus) + E_y_z_15*(g_k_15_16_plus) +
E_y_z_17*(g_k_17_18_plus) E_z_z_13*(g_k_4)];
%---------------------------------------------------------------%
   M_1_trans = M_1'; %NN coupling between A' and B'
   M_1_apostrophe_trans = M_1_apostrophe';
   M_1_apostrophe_1_trans = M_1_apostrophe_1';
%---------------------------------------------------------------%
   H = [M_0 + Delta + M_0_apostrophe + M_0_apostrophe_1 M_1 +
M_1_apostrophe + M_1_apostrophe_1
      M_1_trans + M_1_apostrophe_trans + M_1_apostrophe_1_trans M_0 -
Delta + M_0_apostrophe + M_0_apostrophe_1];
%---------------------------------------------------------------%
   [V,D] = eig(H);
   eigst = sum(D);
   E_2(Nk,:) = sort (real(eigst));
%---------------------------------------------------------------%
end
X_2 = linspace(150, 50, 101);
plot(X_2, E_2 + 3.8, 'k', 'LineWidth', 1.5);
%---------------------------------------------------------------%

%---------------------------------------------------------------%


%------------------M-K (-ve) direction-------------------------%
k_x_3 = linspace(0, (2 * pi)/3/a, 101); k_y = (2 * pi)/sqrt(3)/a; k_z = 0;
for Nk = 1:length(k_x_3)
   k = [k_x_3(Nk) k_y k_z];
%---------------------------------------------------------------%

%-------------Phase factors-------------------------------------%
   g_1_plus = exp(1i*sum(k.*d_1));
   g_2_plus = exp(1i*sum(k.*d_2));
   g_3_plus = exp(1i*sum(k.*d_3));
%---------------------------------------------------------------%
   g_4_plus = exp(1i*sum(k.*d_4));
   g_5_plus = exp(1i*sum(k.*d_5));
   g_6_plus = exp(1i*sum(k.*d_6));
   g_7_plus = exp(1i*sum(k.*d_7));
   g_8_plus = exp(1i*sum(k.*d_8));
   g_9_plus = exp(1i*sum(k.*d_9));
%---------------------------------------------------------------%
   g_10_plus = exp(1i*sum(k.*d_10));
   g_11_plus = exp(1i*sum(k.*d_11));
   g_12_plus = exp(1i*sum(k.*d_12));
%---------------------------------------------------------------%
   g_13_plus = exp(1i*sum(k.*d_13));
   g_14_plus = exp(1i*sum(k.*d_14));
   g_15_plus = exp(1i*sum(k.*d_15));
   g_16_plus = exp(1i*sum(k.*d_16));
   g_17_plus = exp(1i*sum(k.*d_17));
   g_18_plus = exp(1i*sum(k.*d_18));
%---------------------------------------------------------------%
   g_19_plus = exp(1i*sum(k.*d_19));
   g_20_plus = exp(1i*sum(k.*d_20));
   g_21_plus = exp(1i*sum(k.*d_21));
   g_22_plus = exp(1i*sum(k.*d_22));
   g_23_plus = exp(1i*sum(k.*d_23));
   g_24_plus = exp(1i*sum(k.*d_24));
%---------------------------------------------------------------%
   g_k = g_1_plus + g_2_plus + g_3_plus;
   g_k_2_3_minus = g_3_plus - g_2_plus;
   g_k_2_3_plus =  g_3_plus + g_2_plus;
   g_k_3_2_minus = g_2_plus - g_3_plus;
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%---------------------------------------------------------------%
    g_k_2 = g_4_plus + g_5_plus + g_6_plus + g_7_plus + g_8_plus + g_9_plus;
    g_k_4_9 =        g_4_plus - g_5_plus + g_8_plus - g_9_plus;
    g_k_6_7_minus =   g_6_plus - g_7_plus;
    g_k_6_7_plus =    g_6_plus + g_7_plus;
    g_k_4_9_minus =   g_4_plus + g_5_plus - g_8_plus - g_9_plus;
    g_k_4_9_plus =    g_4_plus + g_5_plus + g_8_plus + g_9_plus;
    g_k_4_9_minus_1 = g_4_plus - g_5_plus - g_8_plus + g_9_plus;
%---------------------------------------------------------------%
    g_k_3 = g_10_plus + g_11_plus + g_12_plus;
    g_k_10_11_minus = g_10_plus - g_11_plus;
    g_k_10_11_plus =  g_10_plus + g_11_plus;
%---------------------------------------------------------------%
    g_k_4 = g_13_plus + g_14_plus + g_15_plus + g_16_plus + g_17_plus + g_18_plus;
    g_k_13_14_minus = g_13_plus - g_14_plus;
    g_k_15_16_minus = g_15_plus - g_16_plus;
    g_k_17_18_minus = g_17_plus - g_18_plus;
    g_k_13_14_plus =  g_13_plus + g_14_plus;
    g_k_15_16_plus =  g_15_plus + g_16_plus;
    g_k_16_15_minus = g_16_plus - g_15_plus;
    g_k_17_18_plus =  g_17_plus + g_18_plus;
    g_k_18_17_minus = g_18_plus - g_17_plus;
%---------------------------------------------------------------%
    g_k_5 = g_19_plus + g_20_plus + g_21_plus + g_22_plus + g_23_plus + g_24_plus;
    g_k_19_23_minus =   g_19_plus - g_23_plus;
    g_k_19_23_plus =    g_19_plus + g_23_plus;
    g_k_20_24 =         g_20_plus + g_22_plus - g_21_plus - g_24_plus;
    g_k_20_24_minus =   g_20_plus + g_21_plus - g_22_plus - g_24_plus;
    g_k_20_24_minus_1 = g_20_plus - g_21_plus - g_22_plus + g_24_plus;
    g_k_20_24_plus =    g_20_plus + g_21_plus + g_22_plus + g_24_plus;
%---------------------------------------------------------------%

%-------------Hamiltonian matrix--------------------------------%
    n = 0;
    Delta = n * eye(4);
%---------------------------------------------------------------%
    M_0 = [Epsilon_s 0 0 0
          0 Epsilon_p_x 0 0
          0 0 Epsilon_p_y 0
          0 0 0 Epsilon_p_z]; %On-sites energies of the 4 atomic sites
%---------------------------------------------------------------%
    M_0_apostrophe = [E_s_s_4*(g_k_2) E_s_x_4*(g_k_4_9) + E_s_x_6*(g_k_6_7_minus) E_s_y_4*(g_k_4_9_minus) 0
                   -E_s_x_4*(g_k_4_9) - E_s_x_6*(g_k_6_7_minus) E_x_x_4*(g_k_4_9_plus) + E_x_x_6*(g_k_6_7_plus) E_x_y_4*(g_k_4_9_minus_1) 0
                   -E_s_y_4*(g_k_4_9_minus) E_x_y_4*(g_k_4_9_minus_1) E_y_y_4*(g_k_4_9_plus) + E_y_y_6*(g_k_6_7_plus) 0
                   0 0 0 E_z_z_9*(g_k_2)];
%---------------------------------------------------------------%
    M_0_apostrophe_1 = [E_s_s_19*(g_k_5) E_s_x_20*(g_k_20_24) E_s_y_19*(g_k_19_23_minus) + E_s_y_20*(g_k_20_24_minus) 0
                     -E_s_x_20*(g_k_20_24) E_x_x_19*(g_k_19_23_plus) + E_x_x_20*(g_k_20_24_plus) E_x_y_20*(g_k_20_24_minus_1) 0
                     -E_s_y_19*(g_k_19_23_minus) - E_s_y_20*(g_k_20_24_minus) E_x_y_20*(g_k_20_24_minus_1) E_y_y_19*(g_k_19_23_plus) + E_y_y_20*(g_k_20_24_plus) 0
                     0 0 0 E_z_z_19*(g_k_5)];
%---------------------------------------------------------------%
    M_1 = [E_s_s_1*(g_k) E_s_x_3*(g_k_2_3_minus) E_s_y_1*(g_1_plus) + E_s_y_3*(g_k_2_3_plus) E_s_z_3*(g_k)
        -E_s_x_3*(g_k_2_3_minus) E_x_x_1*(g_1_plus) + E_x_x_3*(g_k_2_3_plus) E_x_y_2*(g_k_3_2_minus) E_x_z_3*(g_k_2_3_minus)
        -E_s_y_1*(g_1_plus) - E_s_y_3*(g_k_2_3_plus) E_x_y_2*(g_k_3_2_minus) E_y_y_1*(g_1_plus) + E_y_y_3*(g_k_2_3_plus) E_y_z_1*(g_1_plus) + E_y_z_3*(g_k_2_3_plus)
        -E_s_z_3*(g_k) E_x_z_3*(g_k_2_3_minus) E_y_z_1*(g_1_plus) + E_y_z_3*(g_k_2_3_plus) E_z_z_1*(g_k)]; %NN coupling between A and B (B' and A')
%---------------------------------------------------------------%
    M_1_apostrophe = [E_s_s_10*(g_k_3) E_s_x_10*(g_k_10_11_minus) E_s_y_10*(g_k_10_11_plus) + E_s_y_12*(g_12_plus) E_s_z_10*(g_k_3)
                   -E_s_x_10*(g_k_10_11_minus) E_x_x_10*(g_k_10_11_plus) + E_x_x_12*(g_12_plus) E_x_y_10*(g_k_10_11_minus) E_x_z_10*(g_k_10_11_minus)
                   -E_s_y_10*(g_k_10_11_plus) - E_s_y_12*(g_12_plus) E_x_y_10*(g_k_10_11_minus) E_y_y_10*(g_k_10_11_plus) + E_y_y_12*(g_12_plus) E_y_z_10*(g_k_10_11_plus) + E_y_z_12*(g_12_plus)
                   -E_s_z_10*(g_k_3) E_x_z_10*(g_k_10_11_minus) E_y_z_10*(g_k_10_11_plus) + E_y_z_12*(g_12_plus) E_z_z_10*(g_k_3)];
%---------------------------------------------------------------%
    M_1_apostrophe_1 = [E_s_s_13*(g_k_4) E_s_x_13*(g_k_13_14_minus) + E_s_x_15*(g_k_15_16_minus) + E_s_x_17*(g_k_17_18_minus) E_s_y_13*(g_k_13_14_plus) + E_s_y_15*(g_k_15_16_plus) + E_s_y_18*(g_k_17_18_plus) E_s_z_13*(g_k_4)
                     -E_s_x_13*(g_k_13_14_minus) - E_s_x_15*(g_k_15_16_minus) - E_s_x_17*(g_k_17_18_minus) E_x_x_13*(g_k_13_14_plus) + E_x_x_15*(g_k_15_16_plus) + E_x_x_18*(g_k_17_18_plus) E_x_y_13*(g_k_13_14_minus) + E_x_y_16*(g_k_16_15_minus) + E_x_y_18*(g_k_18_17_minus) E_x_z_13*(g_k_13_14_minus) + E_x_z_15*(g_k_15_16_minus) + E_x_z_17*(g_k_17_18_minus)
                     -E_s_y_13*(g_k_13_14_plus) - E_s_y_15*(g_k_15_16_plus) - E_s_y_18*(g_k_17_18_plus) E_x_y_13*(g_k_13_14_minus) + E_x_y_16*(g_k_16_15_minus) + E_x_y_18*(g_k_18_17_minus) E_y_y_13*(g_k_13_14_plus) + E_y_y_15*(g_k_15_16_plus) + E_y_y_17*(g_k_17_18_plus) E_y_z_13*(g_k_13_14_plus) + E_y_z_15*(g_k_15_16_plus) + E_y_z_17*(g_k_17_18_plus)
                     -E_s_z_13*(g_k_4) E_x_z_13*(g_k_13_14_minus) + E_x_z_15*(g_k_15_16_minus) + E_x_z_17*(g_k_17_18_minus) E_y_z_13*(g_k_13_14_plus) + E_y_z_15*(g_k_15_16_plus) + E_y_z_17*(g_k_17_18_plus) E_z_z_13*(g_k_4)];
%---------------------------------------------------------------%
    M_1_trans = M_1'; %NN coupling between A' and B'
    M_1_apostrophe_trans = M_1_apostrophe';
    M_1_apostrophe_1_trans = M_1_apostrophe_1';
%---------------------------------------------------------------%
    H = [M_0 + Delta + M_0_apostrophe + M_0_apostrophe_1 M_1 + M_1_apostrophe + M_1_apostrophe_1
        M_1_trans + M_1_apostrophe_trans + M_1_apostrophe_1_trans M_0 - Delta + M_0_apostrophe + M_0_apostrophe_1];
%---------------------------------------------------------------%
    [V,D] = eig(H);
    eigst = sum(D);
    E_3(Nk,:) = sort (real(eigst));
%---------------------------------------------------------------%
end
X_3 = linspace(-0, -50, 101);
plot(-X_3, E_3 + 3.8, 'k', 'LineWidth', 1.5);
%---------------------------------------------------------------%

%---------------------------------------------------------------%

%---------------------------------------------------------------%

%---------------------------------------------------------------%

%---------------------------------------------------------------%

%--------------------Line Demarcations--------------------------%
M = 100;
%---------------------------------------------------------------%
line([150 150], [10 -30], 'Color', 'k', 'LineStyle', '--');
line([50 50], [10 -30], 'Color', 'k', 'LineStyle', '--');
%---------------------------------------------------------------%

%---------------------------------------------------------------%

%---------------Plotting the Fermi level dashed line------------%
fermi_level = 0; % Set the Fermi level value here
fermi_line_x = linspace(0, 250, 101);
fermi_line_y = fermi_level * ones(1, 101);
plot(fermi_line_x, fermi_line_y, 'b--');
%---------------------------------------------------------------%

%--------------------Set x-label ticks--------------------------%
lowerlim = -100;
higherlim = 100;
%---------------------------------------------------------------%
set(gca, 'XTick', [0, higherlim - 50, higherlim + 50, 2 * higherlim + 50]);
set(gca, 'XTickLabel', {'M', 'K', '$\Gamma$', 'M'}, 'Fontsize', 12, 'TickLabelInterpreter', 'latex');
%---------------------------------------------------------------%
xlabel('k-space', 'FontSize', 14, 'FontWeight', 'bold', 'Interpreter', 'latex');
ylabel('Energy band (eV)', 'FontSize', 14, 'FontWeight', 'bold', 'Interpreter', 'latex');
title('5NN (MOTB) Electronic band structure of monolayer blue phosphorene', 'FontSize', 10, 'FontWeight', 'bold', 'Interpreter', 'latex');
%---------------------------------------------------------------%
grid('on');
grid minor;
%---------------------------------------------------------------%
box on;
%---------------------------------------------------------------%

%--------Enhance the quality of the figure----------------------%
set(gcf, 'GraphicsSmoothing', 'on'); %#ok<*SMTHG>
set(gcf, 'Renderer', 'painters');
%---------------------------------------------------------------%

%--------the zoomed-in portion----------------------------------%
xlim([0, 250]);
ylim([-13, 6]);
%---------------------------------------------------------------%
print('TB DFT 5NN MONO LAYER BLUE P.png', '-dpng', '-r600');
%---------------------------------------------------------------%
hold off;
%---------------------------------------------------------------%
```