

or the long wavelength limit ($\vec{q} \rightarrow 0$), we found

$$\vec{P}_{\vec{q}} \sim 0.01e\rho a_0 \hat{e}_z (q_x \cos \phi + q_y \sin \phi) \sim 0.01e\rho a_0 \vec{q} \times \hat{h} \quad (19)$$

where \hat{h} is the helix axis unit vector. We have assumed that $q_z = 0$ since our calculation was performed on xy-plane. If one recognizes that the true meaning of \hat{e}_{12} is the spatial direction along which the spins propagate, i.e., \vec{q} , he can see how the form $\vec{P} \sim eI\hat{e}_{12} \times (\hat{e}_1 \times \hat{e}_2)$ given by KNB can be transformed in the presence of magnetic orders.

0.0.5 5. Discussion

In order to see how magnetic orders and electric order are coupled, let us go back to the original work of Moriya[19]. He derived the following expression:

$$H_{DM} = \sum_N \vec{D}_{N,N-1} \cdot (\vec{S}_N \times \vec{S}_{N-1}) \quad (20)$$

where

$$\vec{D}_{N,N-1} = i\lambda \sum \frac{J(n, n', m, n') \langle n | \vec{l}_i | m \rangle}{E_n - E_m} - i\lambda \sum \frac{J(n, n', n, m') \langle n' | \vec{l}_j | m' \rangle}{E_{n'} - E_{m'}}. \quad (21)$$

Here, $J(n, n', m, m')$ is the exchange interaction strength and \vec{l}_i denotes the angular momentum of the electron at site i .

In our starting Hamiltonian, the exchange interaction comes from the charge transfer energy $\varepsilon_p - \varepsilon_d$ and hybridization energy V [27]. Combined with the spin-orbit interaction in eq. (4b), DM interaction is clearly present in the system we considered. We can recast the wave functions we got previously in a form similar to Moriya's by treating the hybridization energy and spin-orbit interaction as