Theory of antisymmetric spin-pair dependent electric polarization in multiferroics

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We investigate magnetoelectric couplings between an electric polarization and an antisymmetric spin pair $S_i \times S_j$ in a $d$-$p$ model on a distorted lattice based on a perturbation calculation. We microscopically derive a generic form of the antisymmetric spin-pair dependent electric polarization

$$\begin{pmatrix}
  p_{x}^{\text{AS}} \\
  p_{y}^{\text{AS}} \\
  p_{z}^{\text{AS}}
\end{pmatrix} =
\begin{pmatrix}
  d_{xx}^{x} & d_{xy}^{x} & d_{xz}^{x} \\
  d_{yx}^{y} & d_{yy}^{y} & d_{yz}^{y} \\
  d_{zx}^{z} & d_{zy}^{z} & d_{zz}^{z}
\end{pmatrix}
\begin{pmatrix}
  S_{y}^{i} S_{z}^{j} - S_{z}^{i} S_{y}^{j} \\
  S_{z}^{i} S_{x}^{j} - S_{x}^{i} S_{z}^{j} \\
  S_{x}^{i} S_{y}^{j} - S_{y}^{i} S_{x}^{j}
\end{pmatrix}.$$  

On lower symmetry bonds, various elements of the tensor $d$ are non-zero besides the coupling due to the well-known spin-current mechanism. Although the non-spin-current couplings cancel out due to the symmetry on a high symmetry bond, the magnitude of them can be the same order of the spin-current coupling on a lower symmetry bonds. In addition, some of the non-spin-current couplings can be non-uniform on a crystal and thus $p_{\text{AS}}$ shows the possibility that various non-collinear magnetic structures, e.g., canted antiferromagnetic and proper screw states, show multiferroic behaviors as shown in the figure.