

Electric Polarization by Berry Phase: Ver. 1.1

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June 11, 2008

The polarization coming from the electric contribution is given by

$$\mathbf{P} = \sum_{k=1}^3 P_i \mathbf{R}_i. \quad (1)$$

P_i can be evaluated by the following Berry phase formula [1, 2]:

$$\begin{aligned} 2\pi P_i &= \mathbf{G}_i \cdot \mathbf{P} \\ &= -\frac{e}{(2\pi)^3} \sum_{\sigma} \int_{\text{B}} dk^3 \mathbf{G}_i \cdot \left(\frac{\partial}{\partial \mathbf{k}'} \eta_{\sigma}(\mathbf{k}, \mathbf{k}') \right)_{\mathbf{k}'=\mathbf{k}}, \end{aligned} \quad (2)$$

where \int_{B} means that the integral over the first Brillouin zone of which volume is V_{B} . The quantum phase $\eta_{\sigma}(\mathbf{k}, \mathbf{k}')$ is given by

$$\eta_{\sigma}(\mathbf{k}, \mathbf{k}') = \text{Im} \left\{ \ln \left(\det \langle u_{\sigma\mu}^{(\mathbf{k})} | u_{\sigma\nu}^{(\mathbf{k}')} \rangle \right) \right\}, \quad (3)$$

where μ and ν run over the occupied states. The integration and derivative in Eq. (2) are approximated by a discretization:

$$\mathbf{G}_i \cdot \mathbf{P} \approx -\frac{e}{V_{\text{B}} N_2 N_3} \sum_{\sigma} \sum_{i_2=0, i_3=0}^{N_2-1, N_3-1} \sum_{i_1=0}^{N_1-1} \eta_{\sigma}(\mathbf{k}_{i_1 i_2 i_3}, \mathbf{k}'_{i_1+1 i_2 i_3}). \quad (4)$$

Noting that

$$\begin{aligned} \psi_{\sigma\mu}^{(\mathbf{k})}(\mathbf{r}) &= e^{i\mathbf{k}\cdot\mathbf{r}} u_{\sigma\mu}^{(\mathbf{k})}(\mathbf{r}), \\ &= \frac{1}{\sqrt{N}} \sum_{\mathbf{n}} e^{i\mathbf{R}_{\mathbf{n}}\cdot\mathbf{k}} \sum_{i\alpha} c_{\sigma\mu, i\alpha}^{(\mathbf{k})} \phi_{i\alpha}(\mathbf{r} - \tau_i - \mathbf{R}_{\mathbf{n}}), \end{aligned} \quad (5)$$

the overlap matrix $\langle u_{\sigma\mu}^{(\mathbf{k})} | u_{\sigma\nu}^{(\mathbf{k}+\Delta\mathbf{k})} \rangle$ in Eq. (3) is evaluated as

$$\begin{aligned} \langle u_{\sigma\mu}^{(\mathbf{k})} | u_{\sigma\nu}^{(\mathbf{k}+\Delta\mathbf{k})} \rangle &= \langle \psi_{\sigma\mu}^{(\mathbf{k})} | e^{i\mathbf{k}\cdot\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} e^{-i\Delta\mathbf{k}\cdot\mathbf{r}} | \psi_{\sigma\nu}^{(\mathbf{k}+\Delta\mathbf{k})} \rangle, \\ &= \langle \psi_{\sigma\mu}^{(\mathbf{k})} | e^{-i\Delta\mathbf{k}\cdot\mathbf{r}} | \psi_{\sigma\nu}^{(\mathbf{k}+\Delta\mathbf{k})} \rangle, \\ &= \frac{1}{N} \sum_{\mathbf{n}, \mathbf{n}'} \sum_{i\alpha, j\beta} c_{\sigma\mu, i\alpha}^{(\mathbf{k})*} c_{\sigma\nu, j\beta}^{(\mathbf{k}+\Delta\mathbf{k})} e^{-i\mathbf{k}\cdot(\mathbf{R}_{\mathbf{n}} - \mathbf{R}_{\mathbf{n}'})} \times \\ &\quad \langle \phi_{i\alpha}(\mathbf{r} - \tau_i - \mathbf{R}_{\mathbf{n}}) | e^{-i\Delta\mathbf{k}\cdot(\mathbf{r} - \mathbf{R}_{\mathbf{n}'})} | \phi_{j\beta}(\mathbf{r} - \tau_j - \mathbf{R}_{\mathbf{n}'}) \rangle. \end{aligned} \quad (6)$$

Defining that

$$\mathbf{r}' = \mathbf{r} - \tau_i - \mathbf{R}_{\mathbf{n}}, \quad (7)$$

we have

$$\begin{aligned} \langle u_{\sigma\mu}^{(\mathbf{k})} | u_{\sigma\nu}^{(\mathbf{k}+\Delta\mathbf{k})} \rangle &= \frac{1}{N} \sum_{\mathbf{n}, \mathbf{n}'} \sum_{i\alpha, j\beta} c_{\sigma\mu, i\alpha}^{(\mathbf{k})*} c_{\sigma\nu, j\beta}^{(\mathbf{k}+\Delta\mathbf{k})} e^{-i\mathbf{k}\cdot(\mathbf{R}_\mathbf{n}-\mathbf{R}_{\mathbf{n}'})} \times \\ &\quad \langle \phi_{i\alpha}(\mathbf{r}') | e^{-i\Delta\mathbf{k}\cdot(\mathbf{r}'+\tau_i+\mathbf{R}_\mathbf{n}-\mathbf{R}_{\mathbf{n}'})} | \phi_{j\beta}(\mathbf{r}'+\tau_i-\tau_j+\mathbf{R}_\mathbf{n}-\mathbf{R}_{\mathbf{n}'}) \rangle. \end{aligned} \quad (8)$$

Since each term depends on only the relative position $\mathbf{R}_\mathbf{n} - \mathbf{R}_{\mathbf{n}'}$, Eq. (8) becomes

$$\begin{aligned} \langle u_{\sigma\mu}^{(\mathbf{k})} | u_{\sigma\nu}^{(\mathbf{k}+\Delta\mathbf{k})} \rangle &= \sum_{\mathbf{n}} \sum_{i\alpha, j\beta} c_{\sigma\mu, i\alpha}^{(\mathbf{k})*} c_{\sigma\nu, j\beta}^{(\mathbf{k}+\Delta\mathbf{k})} e^{i\mathbf{k}\cdot\mathbf{R}_\mathbf{n}} \times \langle \phi_{i\alpha}(\mathbf{r}') | e^{-i\Delta\mathbf{k}\cdot(\mathbf{r}'+\tau_i-\mathbf{R}_\mathbf{n})} | \phi_{j\beta}(\mathbf{r}'+\tau_i-\tau_j-\mathbf{R}_\mathbf{n}) \rangle, \\ &= \sum_{\mathbf{n}} \sum_{i\alpha, j\beta} c_{\sigma\mu, i\alpha}^{(\mathbf{k})*} c_{\sigma\nu, j\beta}^{(\mathbf{k}+\Delta\mathbf{k})} e^{i\mathbf{k}\cdot\mathbf{R}_\mathbf{n}} e^{-i\Delta\mathbf{k}\cdot(\tau_i-\mathbf{R}_\mathbf{n})} \langle \phi_{i\alpha}(\mathbf{r}') | e^{-i\Delta\mathbf{k}\cdot\mathbf{r}'} | \phi_{j\beta}(\mathbf{r}'+\tau_i-\tau_j-\mathbf{R}_\mathbf{n}) \rangle, \end{aligned} \quad (9)$$

The exponential function in Eq. (9) can be approximated by

$$e^{-i\Delta\mathbf{k}\cdot\mathbf{r}'} \approx 1 - i\Delta\mathbf{k}\cdot\mathbf{r}'. \quad (10)$$

Thus, Eq. (9) becomes

$$\begin{aligned} \langle u_{\sigma\mu}^{(\mathbf{k})} | u_{\sigma\nu}^{(\mathbf{k}+\Delta\mathbf{k})} \rangle &= \sum_{\mathbf{n}} \sum_{i\alpha, j\beta} c_{\sigma\mu, i\alpha}^{(\mathbf{k})*} c_{\sigma\nu, j\beta}^{(\mathbf{k}+\Delta\mathbf{k})} e^{i\mathbf{k}\cdot\mathbf{R}_\mathbf{n}} e^{-i\Delta\mathbf{k}\cdot(\tau_i-\mathbf{R}_\mathbf{n})} \times \\ &\quad \{ \langle \phi_{i\alpha}(\mathbf{r}') | \phi_{j\beta}(\mathbf{r}'+\tau_i-\tau_j-\mathbf{R}_\mathbf{n}) \rangle - i\Delta\mathbf{k}\cdot\langle \phi_{i\alpha}(\mathbf{r}') | \mathbf{r}' | \phi_{j\beta}(\mathbf{r}'+\tau_i-\tau_j-\mathbf{R}_\mathbf{n}) \rangle \}, \end{aligned} \quad (11)$$

where the overlap integral is evaluated in momentum space, and the expectation value for the position operator is evaluated using the same real space mesh as for the solution of Poisson's equation in OpenMX.

References

- [1] R. D. King-Smith, and D. Vanderbilt, Phys. Rev. B **47**, 1651 (1993).
- [2] R. Resta, Rev. Mod. Phys. **66**, 899 (1994).