

# Errata for

## Berry Phases in Electronic Structure Theory: Electric Polarization, Orbital Magnetization and Topological Insulators

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- p. viii: On line 25, “topics topics” should be replaced by “topics”.
- p. 12: Caption of Fig. 1.3: “(a)” should be removed in the first line.
- p. 41: Two lines below Eq. (2.15),  $H_{\text{KS}}$  should be replaced by  $V_{\text{KS}}$ .
- p. 49: Below Eq. (2.45), “any one-particle operator  $\mathcal{O}$ ” should be replaced by “any cell-periodic one-particle operator  $\mathcal{O}$ ”.
- p. 61: Below Eq. (2.75), “secular equation” should be “eigenvalue equation”.
- p. 77: In Eq. (3.3), there is a small right bracket that should be enlarged to match the left bracket.
- p. 86: Exercise 3.2 should read as follows:  
**Exercise 3.2** In Sec. 3.1.1 we constructed the parallel-transport gauge of Eq. (3.9) for the system described by Eq. (3.2). Show that Eq. (3.2) corresponds to a twisted parallel-transport gauge. There are two other choices for a twisted parallel-transport gauge starting from the same  $|\bar{u}_a\rangle$ . What are they?
- p. 86: In Ex. 3.4, “under the cyclic series of distortions shown there” should be replaced by “under the continuous cycle passing through the stages shown there”. In (a), “mesh of  $\varphi$  values and save them in an array” should be replaced by “mesh of  $\varphi$  values, and increase the mesh density until you obtain a converged result”.
- p. 95: On the left-hand side of the last line of (3.43),  $t_{23}$  should be  $t_{20}$ .
- p. 97: On the left-hand side of the last line of (3.44),  $t_{23}$  should be  $t_{20}$ .
- p. 102: In Ex. 3.10(d),  $d\mathbf{d}/dt$  should be  $d\langle\mathbf{d}\rangle/dt$ .
- p. 111: In Ex. 3.11, subscripts  $\mathbf{k}$  should be  $k$  since we are in 1D.
- p. 111: Ex. 3.12(b) should ask to show that  $\bar{\Omega} = \frac{1}{2}\epsilon_{ij}B_{\mu i}B_{\nu j}\Omega_{\mu\nu}$ .

p. 111: In Ex. 3.14(b), `chain.alt_bp` should be `chain.alt_bp.py`.

p. 126: In the first paragraph, the sentence “Expand the set of functions to include the periodic images  $|t_{n\mathbf{R}}\rangle$ , and then construct  $|\chi_{n\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |t_{n\mathbf{R}}\rangle$  in analogy with Eq. (3.80b)” should be replaced by “Construct the band-projected Bloch-like states  $|\chi_{n\mathbf{k}}\rangle = \sum_m |\psi_{m\mathbf{k}}\rangle \langle \psi_{m\mathbf{k}} | t_n \rangle$  at each  $\mathbf{k}$ , where  $m$  runs over occupied Bloch eigenstates”.

p. 127: In the line below Eq. (3.108),  $\langle \tilde{\psi}_{n\mathbf{k}} | H | \tilde{\psi}_{n\mathbf{k}} \rangle$  should be  $\langle \tilde{\psi}_{m\mathbf{k}} | H | \tilde{\psi}_{n\mathbf{k}} \rangle$ .

p. 127: In Eq. (3.112), the factor  $e^{-i\mathbf{k}\cdot\mathbf{R}}$  should be removed.

p. 128: In the first line of the last paragraph, “MLWfs” should be “MLWFs”.

pp. 131-2: The ket  $|\tilde{u}_{nk}\rangle$  should be changed to  $|\tilde{u}'_{nk}\rangle$  in the third line of Sec. 3.6.3, the left-hand side of Eq. (3.123), and in the first and second lines below Eq. (3.123). Similarly, the ket  $|\tilde{u}_{nk_j}\rangle$  should be changed to  $|\tilde{u}'_{nk_j}\rangle$  on the left-hand side of Eq. (3.124), in the top line on p. 132, and in Eq. (3.125).

p. 145: In the last sentence of the first paragraph,  $|\psi_{n\mathbf{k}}(\mathbf{r})|$  should be  $|\psi_{n\mathbf{k}}(\mathbf{r})|^2$ .

p. 149: In Eq. (4.25), the factor of  $2i$  should be replaced by  $-2$  in the second line.

p. 151: In Eq. (4.29), the group velocity vector should be  $\mathbf{v}_{\mathbf{k}}$  (i.e., in bold font).

p. 158: 4.2(b) should be replaced by

Show that  $\langle u_{n\mathbf{k}} | \mathbf{v}_{\mathbf{k}} | u_{n'\mathbf{k}} \rangle = \langle u_{n\mathbf{k}} | \mathbf{p} | u_{n'\mathbf{k}} \rangle / m$  for different bands  $n \neq n'$ .

p. 161: In Eq. (4.51),  $d^3k$  should be replaced by  $d^3\kappa$ .

p. 171: In Eq. (4.69), the prefactor on the right-hand side should be  $e^{i\mathbf{q}\cdot\mathcal{R}_j}$ , not  $e^{i\mathbf{q}\cdot\mathbf{r}_j}$ .

p. 171: Two lines below Eq. (4.69), the text should read “... for a Hamiltonian  $H_{\mathbf{q}} = e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}} H e^{i\mathbf{q}\cdot\hat{\mathbf{r}}}$ , where  $\hat{\mathbf{r}}$  is the coordinate operator; this plays a role ...”.

p. 172: In Ex. 4.8, the displayed equation at the bottom of the page should be

$$p_j = \frac{-e}{2\pi} \bar{\phi}^{(\kappa_j)},$$

and the last text line of the problem on p. 173 should read “as  $p_j = (e/2\pi) \text{Im} \ln \det M$ , where”.

p. 181, Ex. 4.9, the problem should have been posed in the context of the electronic polarization only (i.e., without the ionic contribution).

p. 190: In Eq. (4.93), the sin and cos should be interchanged so that it reads

$$\begin{aligned} \delta &= \delta_0 \sin \lambda, \\ \Delta &= \Delta_0 \cos \lambda, \end{aligned}$$

p. 190: Four lines below Eq. (4.93),  $\delta$  should be  $\delta_0$ .

- p. 203: In the last line of the caption of Fig. 5.1, “ $\mathbf{b}_1$  and  $\mathbf{b}_1$ ” should be “ $\mathbf{b}_1$  and  $\mathbf{b}_2$ ”.
- p. 208: In the 4th line from the top, “ $\mathbb{Z}$  index” should be replaced by “Chern index  $C$ ”.
- p. 209: In the second line of Sec. 5.1.3, “Fig. 5.4(b)” should be “Fig. 5.4(d)”.
- p. 218: In Eq. (5.10), the sum over bands  $n$  should be over all bands.
- p. 219: In the 6th line of the 2nd paragraph,  $\rho_{xx}$  should be  $\sigma_{xx}$ .
- p. 222: In the 8th line of the 2nd paragraph, “It fact” should be “In fact”.
- p. 222: In the last paragraph, the sentence “In Ni the calculated value was only about 30% of the experimental one” should have the words “calculated” and “experimental” interchanged.
- p. 224: In Exercise 5.4 part (c), last sentence, “in part (c)?” should be “in part (b)?”.
- p. 230: On 3rd line from the bottom, “imagin e” should be “imagine”.
- p. 246: In the caption of Fig. 5.17, primed and unprimed indices were interchanged. Thus, the last part of the caption should read:  
 (d)  $\nu_1=1, \nu'_1=0, \nu_2=1, \nu'_2=0$ . (e)  $\nu_1=0, \nu'_1=1, \nu_2=0, \nu'_2=1$ . (f)  $\nu_1=0, \nu'_1=1, \nu_2=1, \nu'_2=0$ .
- p. 247: In the caption of Fig. 5.18, “ $E_{F1}$  and  $E_{F1}$ ” should be “ $E_{F1}$  and  $E_{F2}$ ”.
- p. 250: The sentence ending “approximately 0.3 eV.” in the last paragraph should be followed by “The experimental results are shown in Fig. 5.20.”
- p. 250: There is an erroneous reference to “Xia et al. (2009)” five lines from the bottom of the page. The citation should have been to “Zhang et al. (2009)”.
- p. 252: In Ex. 5.12, “Fig. 5.15(e-g)” should be “Fig. 5.15(e-h)”.
- p. 254: Six lines below Eq. (5.29),  $\sqrt{f_1^2 + f_3^2 + f_3^2}$  should be  $\sqrt{f_1^2 + f_2^2 + f_3^2}$ .
- p. 255: Ten lines above Eq. (5.31), “ $2\pi\chi$ ” should be replaced by “ $\chi$ ”.
- p. 257: The last part of the caption of Fig. 5.22 should read “(a) Positive chirality,  $\chi = +1$ . (b) Negative chirality,  $\chi = -1$ .”
- p. 257: Three lines above Eq. (5.34), the sentence ending “upper bands, respectively” should be extended with “, as shown in Fig. 5.22.”
- p. 260: The sign of  $\chi$  is reversed in several of the lines below Eq. (5.36): in the 4<sup>th</sup> and 11<sup>th</sup> lines,  $-\chi$  should be  $\chi$ ; and in the 12<sup>th</sup> line,  $\chi = C_a - C_b$  should be  $\chi = C_b - C_a$ . (Here Chern indices are defined with respect to the outward normal, unlike in Eq. (5.34).)

- p. 267: Ex. 5.20 should have asked to “show that the AHC is  $\sigma_{\text{AHC}} = -e^2 k_0 / hc$ ”.
- p. 282: In Eqs. (6.16-17), the “Im” should be moved inside the integral for the purposes of Ex. 6.2 on p. 285.
- p. 282: Eq. (6.18) should have  $d^2k$  inserted at the end.
- p. 283: In Eq. (6.22),  $M_{\text{DOS}}$  should be  $\mathbf{M}_{\text{DOS}}$ .
- p. 290: In Fig. 6.5,  $\theta$  should be replaced by  $-\theta$  in the boxed equation at top right.
- p. 293: Eq. (6.32) was missing a factor of  $\mathcal{E}_\nu$ ; it should read
- $$|u_{n\mathbf{k}}\rangle = (1 + i\hbar e \mathcal{E}_\nu T_{n\mathbf{k}}^2 v_{\mathbf{k},\nu}) |u_{n\mathbf{k}}^0\rangle$$
- p. 295: In Eq. (6.42),  $-e$  should be  $-e^2$  in the numerator just after the equal sign.
- p. 296: In Eq. (6.46),  $\tilde{A}$  should be  $\tilde{A}_\mu$ .
- p. 302: In the third line from the bottom of the paragraph beginning “Conversely,” “if is not” should be “if not”.
- p. 304: In the middle paragraph, bold  $\mathbf{k}$  should be italic  $k$  in two places.
- p. 314: In the caption of Fig. 6.9, “electromagnetic” should be “magnetoelectric”.
- p. 328: On the 8th line from the bottom, MATLIB should be MATLAB.
- p. 373: The following item was omitted from the list of references:
- Zhang, H., Liu, C.-X., Qi, X.-L., Dai, X., Fang, Z., and Zhang, S.-C.  
2009. Topological insulators in  $\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  with a single Dirac cone on the surface. *Nat. Phys.* **5**, 438.
- p. 383: In the index entry for “weak index”, the final “ $\mathbb{Z}_2$ ” should be removed.

**To the reader:**

If you discover additional errors, please email [dhv@physics.rutgers.edu](mailto:dhv@physics.rutgers.edu) to report them.

I have also prepared a list of revisions intended to clarify the presentation and provide some missing details. As these go beyond the typical scope of errata, I have provided them separately at <https://www.physics.rutgers.edu/~dhv/book-revisions.pdf>. (If copy-pasting, replace the apparent tilde with a true tilde.)