

# 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. 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: In Ex. 3.14(b), `chain.alt_bp` should be `chain.alt_bp.py`.
- 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.

pp. 131-2: The ket  $|\tilde{u}_{nk}\rangle$  should be changed to  $|\bar{u}'_{nk}\rangle$  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). Also, the ket  $|\tilde{u}_{nk_j}\rangle$  should be changed to  $|\bar{u}'_{nk_j}\rangle$  on the left-hand side of Eq. (3.124) and in the top line on p. 132.

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  $i$  should be deleted from 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. 219: In the 5th 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. 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. 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. 283: In Eq. (6.22),  $M_{\text{DOS}}$  should be  $\mathbf{M}_{\text{DOS}}$ .

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. 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 [www.physics.rutgers.edu/~dhv/book-revisions.pdf](http://www.physics.rutgers.edu/~dhv/book-revisions.pdf).