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

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As of May 12, 2023

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), $H_{KS}$ should be replaced by $V_{KS}$.
p. 49: Below Eq. (2.45), “any one-particle operator $O$” should be replaced by “any
cell-periodic one-particle operator $O$”.
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 $|u_a\rangle$.
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 $k$ 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), $\langle \tilde{\psi}_{nk}|H|\tilde{\psi}_{nk}\rangle$ should be $\langle \tilde{\psi}_{nk}|H|\tilde{\psi}_{nk}\rangle$.
p. 127: In Eq. (3.112), the factor $e^{-ikR}$ should be removed.
p. 128: In the first line of the last paragraph, “MLWFs” should be “MLWFs”.

pp. 131-2: The ket $|\bar{u}_{nk}\rangle$ 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 $|\bar{u}_{nkj}\rangle$ should be changed to $|\bar{u'}_{nkj}\rangle$ 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, $|\psi_{nk}(r)\rangle$ should be $|\psi_{nk}(r)|^2$.

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 $v_k$ (i.e., in bold font).

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

Show that $\langle u_{nk}|v_k|u_{n'k}\rangle = \langle u_{nk}|p|u_{n'k}\rangle/m$ 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 $e^{iq\cdot R_j}$, not $e^{iq\cdot r_j}$.

p. 171: Two lines below Eq. (4.69), the text should read “… for a Hamiltonian $H_q = e^{-iq\cdot \hat{r}}H e^{iq\cdot \hat{r}}$, where $\hat{r}$ 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

$$\delta = \delta_0 \sin \lambda,$$
$$\Delta = \Delta_0 \cos \lambda,$$

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, “$b_1$ and $b_1$” should be “$b_1$ and $b_2$”.

p. 208: In the 4th line from the top, “$Z$ 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 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. 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), $\sqrt{f_1^2 + f_2^2 + f_3^2}$ 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 4th and 11th lines, $-\chi$ should be $\chi$; and in the 12th 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 $\sigma_{AHC} = -e^2 k_0 / hc$.”

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: Eq. (6.18) should have $d^2 k$ inserted at the end.

p. 283: In Eq. (6.22), $M_{DOS}$ should be $M_{DOS}$.

p. 293: Eq. (6.32) was missing a factor of $E_\nu$; it should read
[u_{nk}] = (1 + i\hbar\varepsilon \nu T_{nk}^2 v_{\nu{k',\nu}}) |u_{nk}^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), $\vec{A}$ should be $\vec{A}_{\mu}$.

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 $k$ 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, MATLAB should be MATLAB.

p. 373: The following item was omitted from the list of references:


p. 383: In the index entry for “weak index”, the final “$Z_2$” should be removed.

To the reader:

If you discover additional errors, please email 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.