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), $H_{KS}$ 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 $|\bar{u}_a\rangle$. 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 $k$ 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 $e^{-ik\mathbf{R}}$ should be removed.
In the first line of the last paragraph, “MLWFs” should be “MLWFs”.

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). Also, 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) and in the top line on p. 132.

In the last sentence of the first paragraph, $|\psi_{nk}(r)\rangle$ should be $|\psi_{nk}(r)|^2$.

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

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

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

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

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

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

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

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

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

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

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

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

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

In the last line of the caption of Fig. 5.1, “$b_1$ and $b_1$” should be “$b_1$ and $b_2$”.

In the 4th line from the top, “Z index” should be replaced by “Chern index $C$”.

In the second line of Sec. 5.1.3, “Fig. 5.4(b)” should be “Fig. 5.4(d)”.

In Eq. (5.10), the sum over bands $n$ should be over all bands.

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), $\sqrt{f_1^2 + f_2^3 + f_3^2}$ 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 $\sigma_{AHC} = -e^2 k_0/\hbar c$”.

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 $d^2 k$ 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
\[ |u_{nk}\rangle = (1 + ihe_{\nu}T_{nk}^2v_{k,\nu})|u_{nk}^0\rangle \]

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), \(\tilde{A}\) 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 \(k\) 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, \textsc{matlib} should be \textsc{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.

\textbf{To the reader:}

If you discover additional errors, please email \texttt{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 \texttt{www.physics.rutgers.edu/~dhv/book-revisions.pdf}. 