Errata for

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

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As of November 14, 2021

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 $\mathcal{O}$" 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 φ values and save them in an array" should be replaced by "mesh of φ 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 $\mathbf{v_k}$ (i.e., in bold font).

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

Show that $\langle u_{n\mathbf{k}}|\mathbf{v_k}|u_{n'\mathbf{k}}\rangle = \langle u_{n\mathbf{k}}|\mathbf{p}|u_{n'\mathbf{k}}\rangle/m$ 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 $H_\mathbf{q} = e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}}He^{i\mathbf{q}\cdot\hat{\mathbf{r}}}$, 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 $p_j = (e/2\pi)\,\mathrm{Im}\ln\det M$, 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), δ should be δ_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, ρ_{xx} should be σ_{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 $0.3\,\mathrm{eV}$." 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. 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 χ is reversed in several of the lines below Eq. (5.36): in the 4th and 11th lines, $-\chi$ should be χ; 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 $\sigma_{\mathrm{AHC}} = -e^2 k_0/hc$".

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_{DOS} should be $\mathbf{M}_{\mathrm{DOS}}$.

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), $\widetilde{A}$ should be $\widetilde{A}_\mu$.

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, 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 Bi_2Se_3, Bi_2Te_3 and Sb_2Te_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* 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.*