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. 39: The denominator in Eq. (2.6) should be $|\mathbf{R}_I - \mathbf{R}_J|$.

p. 41: Two lines below Eq. (2.15), $H_{\rm KS}$ should be replaced by $V_{\rm KS}$.

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 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: Ex. 3.12(b) should ask to show that $\overline{\Omega} = \frac{1}{2} \epsilon_{ij} B_{\mu i} B_{\nu j} \Omega_{\mu \nu}$.

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 $|\bar{u}'_{nk}\rangle$ 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 $|\bar{u}_{nk_j}\rangle$ should be changed to $|\bar{u}'_{nk_j}\rangle$ on the right-hand side of Eq. (3.124). Finally, $|\bar{u}_{nk_j}\rangle$ should be changed to $|\tilde{u}_{nk_j}\rangle$ 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 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 $e^{i\mathbf{q}\cdot\mathbf{R}_j}$, 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 $p_j = (e/2\pi)$ 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. 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, 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 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 " χ ".

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 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 $\sigma_{AHC} = -e^2 k_0 / \pi h$ ".

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}_{DOS} .

p. 290: In Fig. 6.5, θ should be replaced by $-\theta$ in the boxed equation at top right.

p. 293: Eq. (6.32) was missing a factor of \mathcal{E}_{ν} ; 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}_{μ} .

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. 307: On this and some subsequent pages, factors of speed of light needed in Gaussian units were omitted. A factor of c should be inserted: (i) p. 307: before $\nabla \times \mathbf{M}$ in Eq. (6.58b) and before $\nabla \times \mathbf{M}_0$ two lines above Eq. (6.61a); (ii) p. 309: before $\mathbf{M} \times \hat{\mathbf{n}}$ eight lines below Eq. (6.63d) and in Fig. 6.6(a); and p. 311, before $\nabla \times \mathbf{M}$ fifteen lines from the bottom of the page and before $\mathbf{M} \times \hat{\mathbf{n}}$ in the following line.

p. 314: In the caption of Fig. 6.9, "electromagnetic" should be "magnetoelectric".

p. 315: Replace " $\mu_0 Q_{\rm m}/4\pi r^2$ " by " $Q_{\rm m}/r^2$ (in Gaussian units)".

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 Bi₂Se₃, Bi₂Te₃ and Sb₂Te₃ 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 $https://www.physics.rutgers.edu/\sim dhv/book-revisions.pdf$. (If copy-pasting, replace the apparent tilde with a true tilde.)