Revisions for

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

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This is a list of intended revisions that go beyond the scope of a simple erratum. These revisions represent attempts to clarify the presentation, or in some cases, to expand the discussion slightly to fill in gaps in the original presentation. In case there is ever an opportunity to publish a second edition of the book, I would expect to include these revisions there.

In what follows, red font is used for new text, and [~~blue~~] is for deleted old text.

List of changes

- p. 69, Eq. (2.88) should be changed to

$$(E_n - H)|\partial_\lambda n\rangle = \big[\partial_\lambda (H - E_n)\big]\,|n\rangle\,. \tag{2.88}$$

  to clarify that the derivative acts only on H and E_n.

- p. 70: Add the following paragraph just above the paragraph containing Eq. (2.92):

  > The preceding expressions are exact at arbitrary λ as long as all relevant quantities (H, $|n\rangle$, E_n, $\mathcal{Q}_n$, etc.) are evaluated at that λ. In practice, however, we typically carry out a perturbation expansion around some λ_0, evaluating all such quantities once and for all at λ_0. In this context we are describing the first order in a perturbation theory in λ.

- p. 70, below Eq. (2.92), modify the text to read

  for any real A_n, as can be checked by plugging into Eq. (2.90)(see Ex. 2.11). [~~and multiplying on the left by an arbitrary eigenstate $\langle m|$ (see Ex. 2.11). In the case that $\langle m| = \langle n|$, this~~] Multiplying both sides of Eq. (2.92) on the left by $\langle n|$ readily yields $\langle n|\partial_\lambda n\rangle = -iA_n$, since ...

- p. 89: Remove the equation number from Eq. (3.35). (See next item.)

- p. 90: Add the following paragraph at the end of Section 3.2.1:

  Note that the Berry curvature of Eq. (3.31) can be written in the notation of Section 2.3 as $-2\mathrm{Im}\,\langle\partial_\mu n|\mathcal{Q}_n|\partial_\nu n\rangle$, where $\mathcal{Q}_n = 1 - |n\rangle\langle n|$ and we have used that $\langle\partial_\mu n|n\rangle = iA_{n,\mu}$ and $\langle n|\partial_\nu n\rangle = -iA_{n,\nu}$ are pure imaginary. Thus, $\Omega_{n,\mu\nu} = -2\mathrm{Im}\,\langle n|(\partial_\mu H)T_n^2(\partial_\nu H)|n\rangle$, or explicitly,

  $$\Omega_{n,\mu\nu} = -2\mathrm{Im}\sum_{m\neq n}\frac{\langle n|(\partial_\mu H)|m\rangle\langle m|(\partial_\nu H)|n\rangle}{(E_n - E_m)^2}\,. \qquad (3.35)$$

  This is sometimes referred to as the "Kubo formula" for the Berry curvature. It is easy to evaluate in a tight-binding context, but requires in principle an infinite sum over unoccupied states in a density-functional context.

- On p. 97, following Ex. 3.5, add a new additional Ex. 3.5a as follows:

  A two-band Hamiltonian that depends on a set of parameters $\boldsymbol{\lambda} = \{\mu, \nu\}$ can always be expanded in Pauli matrices as

  $$h(\boldsymbol{\lambda}) = g(\boldsymbol{\lambda})\mathbb{1}_{2\times 2} + f_1(\boldsymbol{\lambda})\sigma_1 + f_2(\boldsymbol{\lambda})\sigma_2 + f_3(\boldsymbol{\lambda})\sigma_3\,.$$

  Recall that for a 3-vector $\mathbf{f}(\boldsymbol{\lambda})$ depending on two parameters, the solid angle ω spanned by $\mathbf{f}$ on the unit sphere, per unit area in $\boldsymbol{\lambda}$ space, is

  $$\frac{\partial^2\omega}{\partial\mu\partial\nu} = (\partial_\mu\hat{\mathbf{f}})\times(\partial_\mu\hat{\mathbf{f}})\cdot\hat{\mathbf{f}}\,.$$

  Using our standard result for the Berry curvature of a spinor, show that the Berry curvatures of the upper and lower bands (spins pointing along $\pm\hat{\mathbf{f}}$) are given by

  $$\Omega_{\mu\nu}(\boldsymbol{\lambda}) = \mp\frac{(\partial_\mu\mathbf{f})\times(\partial_\mu\mathbf{f})\cdot\mathbf{f}}{2f^3}$$

  respectively. This result is especially relevant to avoided crossings, since the Hamiltonian in the vicinity of an avoided crossing is typically well approximated by considering only the two-band subspace.

- p. 137, above Eq. (3.138), the text should be modified to read

  Let's see how these Berry connection and curvature matrices transform under [~~the~~] a multiband gauge change taking the form of Eq. (3.107). In the present context, $|u_{n\mathbf{k}}\rangle$ and $|\tilde{u}_{n\mathbf{k}}\rangle$ represent two different smooth and periodic choices of gauge. It is useful...

- p. 147, the middle paragraph should be expanded into two paragraphs as follows:

  Recall from Section 2.1.5 that the velocity operator is properly defined as

  $$\mathbf{v} = \frac{-i}{\hbar}\,[\mathbf{r}, H]\,. \tag{4.13}$$

  For a simple Hamiltonian of the form $H = p^2/2m + V(\mathbf{r})$ the velocity operator is just $\mathbf{v} = \mathbf{p}/m$ where m is the electron mass; this simplified expression often appears in the literature. However, we will adopt the proper expression in terms of the commutator above, in part because it must be used in more complicated cases, as when spin-orbit coupling or external fields are present as discussed in Section 2.1.2. For finite systems, Eq. (4.13) leads to the standard identity $i\hbar\langle\psi_m|\mathbf{v}|\psi_n\rangle = (E_n - E_m)\langle\psi_m|\mathbf{r}|\psi_n\rangle$ relating the dipole matrix elements in velocity and position form when taken between two different eigenstates of H.

  Now we heuristically let our finite system become large, identify its eigenstates as Bloch states, and make the transformation from H to $H_\mathbf{k}$ with the corresponding $\mathbf{v}_\mathbf{k} = e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}e^{i\mathbf{k}\cdot\mathbf{r}}$ given by

  $$\mathbf{v}_\mathbf{k} = \frac{-i}{\hbar}\,[\mathbf{r}, H_\mathbf{k}] \tag{4.14}$$

  (since $\mathbf{r}$ commutes with $e^{i\mathbf{k}\cdot\mathbf{r}}$). Then the dipole-matrix-element identity takes the form $i\hbar\langle u_{m\mathbf{k}}|\mathbf{v}_\mathbf{k}|u_{n\mathbf{k}}\rangle = (E_{n\mathbf{k}} - E_{m\mathbf{k}})\langle u_{m\mathbf{k}}|\mathbf{r}|u_{n\mathbf{k}}\rangle$, leading to

  $$\langle u_{m\mathbf{k}}|\mathbf{r}|u_{n\mathbf{k}}\rangle = i\hbar\,\frac{\langle u_{m\mathbf{k}}|\mathbf{v}_\mathbf{k}|u_{n\mathbf{k}}\rangle}{E_{n\mathbf{k}} - E_{m\mathbf{k}}}\,. \tag{4.15}$$

  The right-hand side of this equation remains perfectly well defined in the thermodynamic limit, so we take this as a definition of the expression $\langle u_{m\mathbf{k}}|\mathbf{r}|u_{n\mathbf{k}}\rangle$ (valid only for $m \neq n$) henceforth.

- p. 158, Ex. 4.2: Modify the text to read

  Justify the claim made at the end of Section 4.2.1 to the effect that an electric field perturbation can also be treated as the adiabatic response to a time-dependent vector potential[~~$\mathbf{A}(t) = -c\boldsymbol{\mathcal{E}}t$~~]. Working in 1D, let $A(t) = -c\mathcal{E}t$ (i.e., increasing uniformly with time) and start from Eq. (4.25) with A playing the role of λ. Then use the fact that A and k enter H_k in a similar way to arrive at Eq. (4.22), from which formulas such as Eq. (4.23) follow.

  Note that according to an Erratum, the i should be absent from Eq. (4.25).

- p. 289, just above Eq. (6.27):

In view of this quantum of indeterminacy, it is natural to express α_{iso} in terms of a phase angle θ, known as the "axion angle," defined via

- Sentence crossing from p. 296-7:

  Just as β can be incremented by $2\pi m$ for integer m without changing $e^{-i\beta}$, so can any eigenvalue of B be incremented by $2\pi m$ [~~in the diagonal representation of B~~] (keeping the eigenvectors fixed) without changing U.