Notes on Wannier-interpolated differential operators

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1 Preliminaries

Let $\hat{H}$ be a periodic Hamiltonian with eigenfunctions $|\psi_{n\boldsymbol{k}}\rangle = e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}|u_{n\boldsymbol{k}}\rangle$ and eigenenergies $\epsilon_{n\boldsymbol{k}} = \langle\psi_{n\boldsymbol{k}}|\hat{H}|\psi_{n\boldsymbol{k}}\rangle = \langle u_{n\boldsymbol{k}}|\hat{H}(\boldsymbol{k})|u_{n\boldsymbol{k}}\rangle$. Here, $\hat{H}(\boldsymbol{k}) = e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\hat{H}e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}$ is the Bloch Hamiltonian, and we will define a gauge, $U(\boldsymbol{k})$, of rotated Bloch functions given by $|u_{n\boldsymbol{k}}\rangle = \sum_{n'}|w_{n'\boldsymbol{k}}\rangle U_{nn'}(\boldsymbol{k})$. This gauge is chosen to obtain a set of maximally-localized Wannier functions, given by a Fourier transform as $|n\boldsymbol{R}\rangle = \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}|w_{n\boldsymbol{k}}\rangle$. If $\hat{O}$ is an operator, we denote by $O^H(\boldsymbol{k})$ the matrix elements of $\hat{O}$ in the basis of periodic Bloch functions at fixed $\boldsymbol{k}$, i.e. the Hamiltonian gauge, as $O^H_{nm}(\boldsymbol{k}) = \langle u_{n\boldsymbol{k}}|\hat{O}|u_{m\boldsymbol{k}}\rangle$, and we let $O^W(\boldsymbol{k})$ be the matrix elements in the Wannier gauge, given by $O^W_{nm}(\boldsymbol{k}) = \langle w_{n\boldsymbol{k}}|\hat{O}|w_{m\boldsymbol{k}}\rangle$. Furthermore, by construction $\epsilon_{n\boldsymbol{k}}\delta_{nm} = H^H_{nm}(\boldsymbol{k}) = (U^\dagger(\boldsymbol{k})H^W(\boldsymbol{k})U(\boldsymbol{k}))_{nm}$ and $U(\boldsymbol{k})$ is unitary when $\hat{H}$ is a Hermitian operator. In practice, we evaluate $O^W_{nm}(\boldsymbol{k})$ by Wannier interpolation as $O^W_{nm}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}O^W_{nm\boldsymbol{R}}$ where $O^W_{nm\boldsymbol{R}} = \langle n\boldsymbol{R}|\hat{O}|m\boldsymbol{R}\rangle$.

We say that an operator $\hat{O}$ is gauge-covariant when $O^H(\boldsymbol{k}) = U^\dagger(\boldsymbol{k})O^W(\boldsymbol{k})U(\boldsymbol{k})$ and denote $\bar{O}^H(\boldsymbol{k}) \equiv U^\dagger(\boldsymbol{k})O^W(\boldsymbol{k})U(\boldsymbol{k})$ for further calculation [2].

2 Gauge-covariant derivatives

Let $\hat{O}$ be an operator for which we have a Wannier interpolant, $O^W_{nm}(\boldsymbol{k})$. The interpolant conveniently admits analytic differentiation $\partial_\alpha O^W_{nm}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} iR_\alpha e^{i\boldsymbol{k}\cdot\boldsymbol{R}}O^W_{nm\boldsymbol{R}}$. Here, we abbreviate $\partial_\alpha \equiv \frac{\partial}{\partial k_\alpha}$. Note also that $\partial_\alpha O^W_{nm}(\boldsymbol{k}) = \partial_\alpha\langle w_{n\boldsymbol{k}}|\hat{O}|w_{m\boldsymbol{k}}\rangle = \langle w_{n\boldsymbol{k}}|\partial_\alpha\hat{O}|w_{m\boldsymbol{k}}\rangle + \langle\partial_\alpha w_{n\boldsymbol{k}}|\hat{O}|w_{m\boldsymbol{k}}\rangle + \langle w_{n\boldsymbol{k}}|\hat{O}|\partial_\alpha w_{m\boldsymbol{k}}\rangle$. By resolving the identity, $I = \sum_n |w_{n\boldsymbol{k}}\rangle\langle w_{n\boldsymbol{k}}|$, defining the Berry connection, $A^W_{nm\alpha}(\boldsymbol{k}) = i\,\langle w_{n\boldsymbol{k}}|\partial_\alpha w_{m\boldsymbol{k}}\rangle$, and using the orthonormality of the $|w_{n\boldsymbol{k}}\rangle$, we may write

$$(\partial_\alpha O)^W_{nm}(\boldsymbol{k}) \equiv \langle w_{n\boldsymbol{k}}|\partial_\alpha \hat{O}|w_{m\boldsymbol{k}}\rangle = \partial_\alpha O^W_{nm}(\boldsymbol{k}) + i[O^W(\boldsymbol{k}), A^W_\alpha(\boldsymbol{k})]_{nm}. \tag{1}$$

An analogous formula exists in any gauge, with its own respective Berry connection. By construction, $(\partial_\alpha O)^W(\boldsymbol{k})$ is gauge-covariant, so we call it a gauge-covariant derivative (notice the ∂_α symbol is inside the matrix element, not outside). However, it can be shown that $A^W_\alpha(\boldsymbol{k})$ is not gauge-covariant, since

$$\begin{aligned} A^H_{nm\alpha}(\boldsymbol{k}) &= i\,\langle u_{n\boldsymbol{k}}|\partial_\alpha u_{m\boldsymbol{k}}\rangle\,, & (2)\\ &= i\left\langle \sum_{n'} |w_{n'\boldsymbol{k}}\rangle\, U_{nn'}(\boldsymbol{k}) \middle| \partial_\alpha \sum_{m'} |w_{m'\boldsymbol{k}}\rangle\, U_{mm'}(\boldsymbol{k}) \right\rangle, & (3)\\ &= (U^\dagger(\boldsymbol{k}) A^W_\alpha(\boldsymbol{k}) U(\boldsymbol{k}) + iU^\dagger(\boldsymbol{k})\partial_\alpha U(\boldsymbol{k}))_{nm}, & (4)\\ &= (\bar{A}^H_\alpha(\boldsymbol{k}) + iU^\dagger(\boldsymbol{k})\partial_\alpha U(\boldsymbol{k}))_{nm}. & (5) \end{aligned}$$

Ref. [1] defines $D_\alpha(\boldsymbol{k}) \equiv U^\dagger(\boldsymbol{k})\partial_\alpha U(\boldsymbol{k})$ and obtains its matrix elements in the Hamiltonian gauge using first order perturbation theory,

$$D^H_{nm\alpha}(\boldsymbol{k}) = (U^\dagger(\boldsymbol{k})\partial_\alpha U(\boldsymbol{k}))_{nm} = \begin{cases} (U^\dagger(\boldsymbol{k})\partial_\alpha H^W(\boldsymbol{k}) U(\boldsymbol{k}))_{nm}/(\epsilon_{m\boldsymbol{k}} - \epsilon_{n\boldsymbol{k}}) & n \neq m \\ 0 & n = m \end{cases}. \tag{6}$$

Note that this definition does not use the gauge-covariant derivative, so to me it is unclear which operator is the perturbation to the Hamiltonian, although below it will be clear this gives a consistent definition of the velocity.

3 Example: velocity operator

The velocity operator can be defined by $\hat{v}_\alpha = -i[\hat{r}_\alpha, \hat{H}] = \partial_\alpha \hat{H}(\boldsymbol{k})$, ($\hbar = 1$). Semi-classically, the group velocity is simply $v_{n\boldsymbol{k}\alpha} = \partial_\alpha \epsilon_{n\boldsymbol{k}}$. To obtain this in the Wannier gauge, we start from (1) in the Hamiltonian gauge:

$$\begin{aligned} \partial_\alpha \epsilon_{n\boldsymbol{k}} \delta_{nm} &= \partial_\alpha H^H_{nm}(\boldsymbol{k}) = \langle u_{n\boldsymbol{k}}|\partial_\alpha \hat{H}|u_{m\boldsymbol{k}}\rangle - i[H^H(\boldsymbol{k}), A^H_\alpha(\boldsymbol{k})]_{nm} & (7)\\ &= (U^\dagger(\boldsymbol{k})(\partial_\alpha H^W(\boldsymbol{k}) + i[H^W(\boldsymbol{k}), A^W_\alpha(\boldsymbol{k})])U(\boldsymbol{k}) - i[U^\dagger(\boldsymbol{k})H^W(\boldsymbol{k})U(\boldsymbol{k}), A^H_\alpha(\boldsymbol{k})])_{nm} & (8)\\ &= (U^\dagger(\boldsymbol{k})\partial_\alpha H^W(\boldsymbol{k})U(\boldsymbol{k}) + [U^\dagger(\boldsymbol{k})H^W(\boldsymbol{k})U(\boldsymbol{k}), D^H_\alpha(\boldsymbol{k})])_{nm} & (9) \end{aligned}$$

In the final expression, the off-diagonal elements cancel with the commutator, which is purely off-diagonal (since H^H is diagonal) given the above definition of D_α. This leaves only the diagonal elements of the first term, which correctly match the derivatives of the eigenvalues.

4 Example: inverse effective mass

We can conveniently define a second derivative operator $-i[\hat{r}_\alpha, \hat{v}_\beta] = -[\hat{r}_\alpha, [\hat{r}_\beta, \hat{H}]] = \partial^2_{\alpha\beta}\hat{H}(\boldsymbol{k})$. This can also take a gauge-covariant form:

$$
\begin{aligned}
(\partial^2_{\alpha\beta}H)^W_{nm}(\boldsymbol{k}) = (\partial_\alpha v_\beta)^W_{nm}(\boldsymbol{k}) &= \partial_\alpha v^W_{nm\beta}(\boldsymbol{k}) + i[v^W_\beta(\boldsymbol{k}), A^W_\alpha(\boldsymbol{k})]_{nm} && (10)\\
&= \partial^2_{\alpha\beta}H^W_{nm}(\boldsymbol{k}) + i\partial_\alpha[H^W(\boldsymbol{k}), A^W_\beta(\boldsymbol{k})]_{nm} && (11)\\
&+ i[\partial_\beta H^W(\boldsymbol{k}) + i[H^W(\boldsymbol{k}), A^W_\beta(\boldsymbol{k})], A^W_\alpha(\boldsymbol{k})]_{nm} && (12)
\end{aligned}
$$

However, the inverse effective mass is defined as a second derivative of an eigenvalue, $\partial^2_{\alpha\beta}\epsilon_{n\boldsymbol{k}} = \partial_\alpha \langle u_{n\boldsymbol{k}}|\hat{v}_\beta|u_{n\boldsymbol{k}}\rangle = \langle u_{n\boldsymbol{k}}|\partial_\alpha\hat{v}_\beta|u_{n\boldsymbol{k}}\rangle - i[v^H_\beta(\boldsymbol{k}), A^H_\alpha(\boldsymbol{k})]_{nn} = (U^\dagger(\boldsymbol{k})(\partial_\alpha v^W_\beta(\boldsymbol{k}) + i[v^W_\beta(\boldsymbol{k}), A^W_\alpha(\boldsymbol{k})])U(\boldsymbol{k}))_{nn} - i[v^H_\beta(\boldsymbol{k}), A^H_\alpha(\boldsymbol{k})]_{nn}$ where we have used the Hellman-Feynman theorem to obtain the second expression. Alternatively, as in Ref. [2], we may write $\partial_\alpha \langle u_{n\boldsymbol{k}}|\hat{v}_\beta|u_{n\boldsymbol{k}}\rangle = \partial_\alpha(\langle u_{n\boldsymbol{k}}|w_{m\boldsymbol{k}}\rangle \langle w_{m\boldsymbol{k}}|\hat{v}_\beta|w_{l\boldsymbol{k}}\rangle \langle w_{l\boldsymbol{k}}|u_{n\boldsymbol{k}}\rangle) = (U^\dagger(\boldsymbol{k})\partial_\alpha v^W_\beta(\boldsymbol{k})U(\boldsymbol{k}) + \{\partial_\alpha U^\dagger(\boldsymbol{k})U(\boldsymbol{k})U^\dagger(\boldsymbol{k})v^W_\beta(\boldsymbol{k})U(\boldsymbol{k}) + \text{h.c.}\})_{nn}$. This latter formula is consistent with the former given and the way the Berry connection transforms from Wannier to Hamiltonian gauge.

References

[1] Xinjie Wang et al. "Ab Initio Calculation of the Anomalous Hall Conductivity by Wannier Interpolation". In: *Physical Review B* 74.19 (Nov. 21, 2006), p. 195118. DOI: `10.1103/PhysRevB.74.195118`. URL: `https://link.aps.org/doi/10.1103/PhysRevB.74.195118` (visited on 08/02/2023).

[2] Jonathan R. Yates et al. "Spectral and Fermi Surface Properties from Wannier Interpolation". In: *Physical Review B* 75.19 (May 21, 2007), p. 195121. DOI: `10.1103/PhysRevB.75.195121`. URL: `https://link.aps.org/doi/10.1103/PhysRevB.75.195121` (visited on 02/23/2022).