Comment on the calculation of the second band derivative at degeneracy points in the BZ

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1 Background

In Ref. [1], the authors propose a first principles method based on the theory of Maximally Localized Wannier Functions (MLWFs) [2] to calculate some crystal properties in reciprocal space.

This document is concerned with some statements made on Sec. II C 4, regarding the calculation of the so-called inverse mass tensor $\mu_{n,\alpha\beta}(\boldsymbol{k})$ on the $\boldsymbol{k}$ points in which the bands are degenerate. In the following we reproduce the results from Ref. [1], which hold for any $\boldsymbol{k}$ point yielding a nondegenerate band structure:

$$\begin{aligned}
\mu_{n,\alpha\beta} &= \left[\bar{H}^{(H)}_{\alpha\beta} + \left\{\bar{H}^{(H)}_{\alpha} D^{(H)}_{\beta} + \text{H.c.}\right\}\right]_{nn} \\
\bar{O}^{(H)} &= U^{\dagger} O^{(W)} U \\
\bar{O}^{(H)}_{\alpha} &= U^{\dagger} \frac{\partial O^{(W)}}{\partial k_\alpha} U \\
\bar{O}^{(H)}_{\alpha\beta} &= U^{\dagger} \frac{\partial^2 O^{(W)}}{\partial k_\alpha \partial k_\beta} U \\
D^{(H)}_{nm,\beta} &= \left(U^{\dagger}\frac{\partial U}{\partial k_\beta}\right)_{nm} = \begin{cases} \frac{\bar{H}^{(H)}_{nm,\beta}}{\varepsilon_m - \varepsilon_n}, & \text{if} \quad n \neq m \\ 0, & \text{if} \quad n = m \end{cases}
\end{aligned} \tag{1}$$

Where $O^{(W)}$ is a general $M \times M$ matrix representing the operator $\hat{O}$ in the Wannier *gauge* and point $\boldsymbol{k}$, which is given by

$$O^{(W)}_{nm}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle n\mathbf{0}|\hat{O}|m\boldsymbol{R}\rangle \,. \tag{2}$$

2 Problem Statement

In Sec. II C 4, emphasis is made on how standard perturbation theory [3, 4] can be applied to obtain sensible results from Eq.(1) at those $\boldsymbol{k}$ points in which the band structure is degenerate. The method proposes to change the matrix U, updating the matrix elements from the restriction corresponding to the degenerate band subspace by those eigenvectors diagonalizing $\bar{H}^{(H)}_{\beta}$ in the same subspace[1]. We believe that the authors made a mistake and mistook the matrix U for the matrix D_β, since the matrix U is related to the *gauge* freedom in the definition of the MLWFs $|n\boldsymbol{R}\rangle$, which is fixed by minimizing the spread functional [2] and it is not directly tied to the points in which the band structure becomes degenerate.

Our main argument is that in Ref. [5], where the matrix $D^{(H)}_{\beta}$ was first defined, perturbation theory was employed to obtain the expression on Eq. (1) (see Eq. (22) and Eq. (24) of Ref. [5]). The reader may recognize the definition given for $D^{(H)}_{\beta}$ as the first-order eigenvalue correction in the perturbation expansion corresponding to a nondegenerate level [3]. As such, $D^{(H)}_{\beta}$ becomes ill defined whenever $\varepsilon_n = \varepsilon_m$ for $n \neq m$.

[1] If the eigenvalues are given by an array ε_i and say, that N levels are degenerate starting from index j, then the U matrix elements from j to $j+N-1$ must be updated by the eigenvectors diagonalizing the submatrix $\bar{H}^{(H)}_{nm,\beta},\ n,m = j,\cdots,j+N-1$.

3 Proposed Solution

Since $D_\beta^{(H)}$ is ill defined on degeneracy points, degenerate perturbation theory must be used to obtain sensible results. This is done by using the eigenvectors diagonalizing $\bar{H}_\beta^{(H)}$ on the degenerate subspace to replace the matrix elements of $D_\beta^{(H)}$ on the same subspace.

References

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