Inversion Symmetry and Wannier States

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1 Example 1

Consider a one-dimensional system with two localized orbitals centered at the unit-cell center, both having positive inversion eigenvalue. See Fig. 1(a). The inversion action is

$$\hat{I}\,|w_{1,R}\rangle = |w_{1,-R}\rangle\,, \quad \hat{I}\,|w_{2,R}\rangle = |w_{2,-R}\rangle\,. \tag{1}$$

Let the corresponding Bloch states be

$$|\phi_{j,k}\rangle = \sum_R |w_{j,R}\rangle\, e^{ikR}, \quad j = 1, 2, \tag{2}$$

and write

$$\Phi_k = (|\phi_{1,k}\rangle\,, |\phi_{2,k}\rangle). \tag{3}$$

Then inversion acts on Φ_k as

$$\hat{I}\Phi_k = \Phi_{-k} I_k, \quad I_k = 1_2. \tag{4}$$

If inversion symmetry is ignored, the two localized orbitals can be hybridized so that they become localized at $x = a$ and $x = -a$. Concretely, redefine

$$\Phi'_k = (\phi'_{1,k}, \phi'_{2,k}) = \Phi_k U_k = \Phi_k \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2}e^{ik} \\ \sin\frac{\theta}{2}e^{-ik} & \cos\frac{\theta}{2} \end{pmatrix}. \tag{5}$$

The centers, equivalently the Berry phases, of the Wannier states constructed from $\phi'_{1,k}, \phi'_{2,k}$,

$$|w'_{j,R}\rangle = \sum_k |\phi'_{j,k}\rangle\, e^{-ikR}, \quad j = 1, 2, \tag{6}$$

are

$$r'_j = \langle w'_{j,R=0}|\hat{r}|w'_{j,R=0}\rangle\,, \tag{7}$$

and change as

$$r'_1 = \sin^2\frac{\theta}{2}, \quad r'_2 = -\sin^2\frac{\theta}{2}. \tag{8}$$

Indeed, the Wannier states transform as

$$|w'_{1,R}\rangle = \cos\frac{\theta}{2}\,|w_{1,R}\rangle + \sin\frac{\theta}{2}\,|w_{2,R+1}\rangle\,, \tag{9}$$

$$|w'_{2,R}\rangle = -\sin\frac{\theta}{2}\,|w_{1,R-1}\rangle + \cos\frac{\theta}{2}\,|w_{2,R}\rangle\,, \tag{10}$$

and using $\hat{r}\,|w_{j,R}\rangle = R\,|w_{j,R}\rangle$ reproduces the calculation above.

In the basis Φ'_k, the representation matrix of inversion is

$$\hat{I}\Phi'_k = \hat{I}\Phi_k U_k = \Phi_{-k} I_k U_k = \Phi'_{-k} U^\dagger_{-k} I_k U_k, \tag{11}$$

so

$$I'_k = U^\dagger_{-k} I_k U_k = \begin{pmatrix} \cos^2\frac{\theta}{2} + e^{-2ik}\sin^2\frac{\theta}{2} & i\sin k\sin\theta \\ i\sin k\sin\theta & \cos^2\frac{\theta}{2} + e^{2ik}\sin^2\frac{\theta}{2} \end{pmatrix}. \tag{12}$$

Write

$$W'_R = (|w'_{1,R}\rangle, |w'_{2,R}\rangle). \tag{13}$$

The inversion action on Wannier states is

$$\hat{I}W'_R = \sum_{R'} W'_{R'} \sum_k I'_k e^{ik(R-R')}. \tag{14}$$

Thus it is determined by

$$I'_{R-R'} = \sum_k I'_k e^{ik(R-R')}. \tag{15}$$

A direct computation gives

$$I'_{R-R'} = \begin{cases} \begin{pmatrix} \cos^2\frac{\theta}{2} & \\ & \cos^2\frac{\theta}{2} \end{pmatrix} & (R-R'=0), \\ \begin{pmatrix} & \pm\frac{1}{2}\sin\theta \\ \pm\frac{1}{2}\sin\theta & \end{pmatrix} & (R-R'=\pm 1), \\ \begin{pmatrix} \sin^2\frac{\theta}{2} & \\ & 0 \end{pmatrix} & (R-R'=2), \\ \begin{pmatrix} 0 & \\ & \sin^2\frac{\theta}{2} \end{pmatrix} & (R-R'=-2), \\ O & (\text{otherwise}). \end{cases} \tag{16}$$

Hence the action does not close within a single Wannier state at a fixed site R. If one restricts to gauge transformations of the form (5), one also checks that closure occurs only for $\theta = 0$, namely for the original Wannier states $|w_{1,R}\rangle, |w_{2,R}\rangle$.

- Is there another gauge transformation, other than (5), for which $r'_1 = -r'_2 = a \neq 0$ and inversion symmetry closes on one or two Wannier states, meaning that the relevant matrix elements of $I'_{R-R'}$ have absolute value 1?

2 Example 2

Now consider two localized orbitals centered at the unit-cell center, but with opposite inversion eigenvalues, positive and negative. See Fig. 1(b). The action is

$$\hat{I}|w_{1,R}\rangle = |w_{1,-R}\rangle, \quad \hat{I}|w_{2,R}\rangle = -|w_{2,-R}\rangle. \tag{17}$$

Accordingly,

$$I_k = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}. \tag{18}$$

Within the space spanned by $|w_{1,R}\rangle, |w_{2,R}\rangle$, the inversion matrix is unitarily equivalent to

$$I \sim \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}. \tag{19}$$

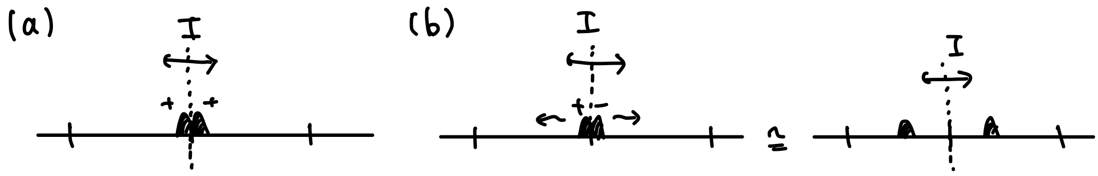

Figure 1:

In such a basis, the Wannier centers can be continuously moved to $x = a$ and $x = -a$ while preserving inversion symmetry. Therefore one expects that a suitable gauge of Φ_k can be chosen so that $r_1 = -r_2 = a$ and

$$I_k = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}. \tag{20}$$

Writing out the conditions, we seek a gauge transformation

$$U_k = \begin{pmatrix} u_k & -v_k^* \\ v_k & u_k^* \end{pmatrix} \tag{21}$$

such that

$$I_k' = U_{-k}^\dagger I_k U_k = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} \tag{22}$$

and the Berry phase

$$r_1' = \frac{i}{2\pi} \oint_0^{2\pi} dk\, (u_k^* \partial u_k + v_k^* \partial v_k) \tag{23}$$

is nonzero.

Without deriving the general solution, we show that a nontrivial solution exists. Take

$$U_k = \begin{pmatrix} \frac{\cos(\theta/2)+\sin(\theta/2)(i\cos k+\sin k)}{\sqrt{2}} & \frac{\cos(\theta/2)+ie^{ik}\sin(\theta/2)}{\sqrt{2}} \\ \frac{\cos(\theta/2)-ie^{-ik}\sin(\theta/2)}{\sqrt{2}} & \frac{ie^{ik}\sin(\theta/2)-\cos(\theta/2)}{\sqrt{2}} \end{pmatrix}. \tag{24}$$

This satisfies the required conditions and gives

$$r_1' = \sin^2 \frac{\theta}{2}. \tag{25}$$

- In general, if an adiabatic deformation of an atomic insulator exists, does the corresponding gauge transformation $U_{\boldsymbol{k}}$ also exist?
- Can the condition that Wannier states form a "space-group-symmetric atomic insulator" be defined by requiring that the transition matrices between Wannier states,

$$U_g(\boldsymbol{R} - \boldsymbol{R}') = \int_{T^3} \frac{d^3k}{(2\pi)^3} U_g(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}, \tag{26}$$

constructed from the space-group symmetry operator $U_g(\boldsymbol{k})$, agree with the matrix elements of a space-group representation induced from some atomic insulator? Is there a cleaner definition?