Floquet TI calculations

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III. Calculation of Floquet bands for a Dirac band

For the two dimensional Dirac band, the hamiltonian is[1]

$$H(t) = \tau_z v[k^x + A^x_{ac}(t)]\sigma_x + v[k^y + A^y_{ac}(t)]\sigma_y.$$

$\tau_z = \pm 1$ is a generalized "valley" index, v is the velocity, and $\vec{\sigma}$ are the Pauli matrices. The Schrodinger equation reads

$$H(t)\left|\Psi_\alpha(t)\right\rangle = i\frac{\partial}{\partial t}\left|\Psi_\alpha(t)\right\rangle.$$

This may be rearranged using the notation of Floquet theory; introduce $\mathcal{H}(t) = H(t) - i\partial_t$ to obtain

$$\mathcal{H}(t)\left|\Psi_\alpha t\right\rangle = 0.$$

Floquet's theorem (equivalent to Bloch's theorem for spatially periodic systems) says that for time periodic $H(t)$ (in this case, time-periodic A_{ac}), there exists a set of states $\left|\Phi_\alpha(t)\right\rangle$ which are periodic:

$$\left|\Phi_\alpha(t+T)\right\rangle = \left|\Phi_\alpha(t)\right\rangle,$$

and which satisfy the Floquet equation:

$$\mathcal{H}(t)\left|\Phi_\alpha(t)\right\rangle = \epsilon_\alpha\left|\Phi_\alpha(t)\right\rangle,$$

where ϵ_α are known as quasienergies.

Now express the "Floquet functions"[2] by their Fourier components:

$$\left|\Phi_\alpha(t)\right\rangle = \sum_m e^{-im\Omega t}\left|u^m_\alpha\right\rangle,$$

for some kets $|u\rangle$.

Re-expanding the Floquet operator $\mathcal{H}$ in terms of H and ∂_t gives

$$\sum_m H(t)e^{-im\Omega t}\left|u^m_\alpha\right\rangle = \sum_m \left[\epsilon_\alpha + m\Omega\right]e^{-im\Omega t}\left|u^m_\alpha\right\rangle$$

Choose A to be a circularly polarized field: $\vec{A} = A(\cos\Omega t, \sin\Omega t)$. Here, $A = F/\Omega$ and F is the "field strength."[3] Then the equation reads

$$\sum_m \left\{\tau_z v[k^x + A\cos\Omega t]\sigma_x + v[k^y + A\sin\Omega t(t)]\sigma_y\right\}e^{-im\Omega t}\left|u^m_\alpha\right\rangle = \sum_m \left[\epsilon_\alpha + m\Omega\right]e^{-im\Omega t}\left|u^m_\alpha\right\rangle.$$

[1] firt paragraph, section 3
[2] by analogy with Bloch functions??
[3] ?? units

Integration against $e^{in\Omega t}$ yields

$$\sum_m \frac{1}{T}\int_0^T dt\ \{\tau_z v[k^x + A\cos\Omega t]\sigma_x + v[k^y + A\sin\Omega t(t)]\sigma_y\}\, e^{-i(m-n)\Omega t}\,|u_\alpha^m\rangle$$
$$= \sum_m \frac{1}{T}\int_0^T dt\ [\epsilon_\alpha + m\Omega]\, e^{-i(m-n)\Omega t}\,|u_\alpha^m\rangle$$

The needed integrals are

$$\begin{aligned}\frac{1}{T}\int_0^T dt\ \cos\Omega t\, e^{-i(m-n)\Omega t} &= \frac{1}{2T}\int_0^T dt\ \left(e^{i(n-m+1)\Omega t} + e^{i(n-m-1)\Omega t}\right)\\ &= \frac{1}{2}\left(\delta_{m,n+1} + \delta_{m,n-1}\right)\end{aligned}$$

$$\begin{aligned}\frac{1}{T}\int_0^T dt\ \sin\Omega t\, e^{-i(m-n)\Omega t} &= \frac{1}{2iT}\int_0^T dt\ \left(e^{i(n-m+1)\Omega t} - e^{i(n-m-1)\Omega t}\right)\\ &= \frac{1}{2i}\left(\delta_{m,n+1} - \delta_{m,n-1}\right)\end{aligned}$$

The Fourier-transformed Floquet equation becomes

$$\sum_m \left\{\tau_z v\left[k^x\delta_{m,n} + \frac{1}{2}A(\delta_{m,n+1}+\delta_{m,n-1})\right]\sigma_x + v\left[k^y + \frac{1}{2i}A(\delta_{m,n+1}-\delta_{m,n-1})\right]\sigma_y\right\}$$
$$= \sum_m [\epsilon_\alpha + m\Omega]\,\delta_{m,n}\,|u_\alpha^m\rangle$$

$$\Rightarrow \left[(\tau_z v k^x\sigma_x + v k^y\sigma_y)\,|u_\alpha^n\rangle + \frac{1}{2}Av(\tau_z\sigma_x - i\sigma_y)\,|u_\alpha^{n+1}\rangle + \frac{1}{2}Av(\tau_z\sigma_x + i\sigma_y)\,|u_\alpha^{n-1}\rangle\right] = [\epsilon_\alpha + n\Omega]\,|u_\alpha^n\rangle$$

The left-hand side can be written in the form of a tridiagonal matrix, since the n component is linked to $n-1$ and $n+1$. The nth block of this matrix looks like

$$\begin{pmatrix} v(k^x\tau_z\otimes\sigma_x + k^y 1\otimes\sigma^y) & \frac{1}{2}Av(\tau_z\otimes\sigma_x + i1\otimes\sigma_y) & 0\\ \frac{1}{2}Av(\tau_z\otimes\sigma_x - i1\otimes\sigma_y) & v(k^x\tau_z\otimes\sigma_x + k^y 1\otimes\sigma^y) & \frac{1}{2}Av(\tau_z\otimes\sigma_x + i1\otimes\sigma_y)\\ 0 & \frac{1}{2}Av(\tau_z\otimes\sigma_x - i1\otimes\sigma_y) & v(k^x\tau_z\otimes\sigma_x + k^y 1\otimes\sigma^y)\end{pmatrix}.$$

It is easiest to study the τ_z bands separately. First takes $\tau_z = +1$. This sector of the matrix takes the form

$$(\tau_z\otimes\sigma_x - i1\otimes\sigma_y) \to \begin{pmatrix} 0 & 0\\ 2 & 0\end{pmatrix},$$

$$(\tau_z\otimes\sigma_x + i1\otimes\sigma_y) \to \begin{pmatrix} 0 & 2\\ 0 & 0\end{pmatrix},$$

$$(k^x\tau_z\otimes\sigma_x + k^y 1\otimes\sigma^y) \to \begin{pmatrix} 0 & k^x - ik^y\\ k^x + ik^y & 0\end{pmatrix}.$$

On the other hand, the $\tau_z = -1$ sector gives

$$(\tau_z\otimes\sigma_x - i1\otimes\sigma_y) \to \begin{pmatrix} 0 & -2\\ 0 & 0\end{pmatrix},$$

$$(\tau_z\otimes\sigma_x + i1\otimes\sigma_y) \to \begin{pmatrix} 0 & 0\\ -2 & 0\end{pmatrix},$$

$$(k^x \tau_z \otimes \sigma_x + k^y 1 \otimes \sigma^y) \to \begin{pmatrix} 0 & k^x - ik^y \\ k^x + ik^y & 0 \end{pmatrix}.$$

Setting $v = 1$, this block of the matrix equation takes the forms

$$\tau_z = +1 : \begin{pmatrix} -(n-1)\Omega & k^x - ik^y & 0 & A & 0 & 0 \\ k^x + ik^y & -(n-1)\Omega & 0 & 0 & 0 & 0 \\ 0 & 0 & -n\Omega & k^x - ik^y & 0 & A \\ A & 0 & k^x + ik^y & -n\Omega & 0 & 0 \\ 0 & 0 & 0 & 0 & -(n+1)\Omega & k^x - ik^y \\ 0 & 0 & A & 0 & k^x + ik^y & -(n+1)\Omega \end{pmatrix}$$

$$\tau_z = -1 : \begin{pmatrix} -(n-1)\Omega & k^x - ik^y & 0 & 0 & 0 & 0 \\ k^x + ik^y & -(n-1)\Omega & -A & 0 & 0 & 0 \\ 0 & -A & -n\Omega & k^x - ik^y & 0 & 0 \\ 0 & 0 & k^x + ik^y & -n\Omega & -A & 0 \\ 0 & 0 & 0 & -A & -(n+1)\Omega & k^x - ik^y \\ 0 & 0 & 0 & 0 & k^x + ik^y & -(n+1)\Omega \end{pmatrix}$$