2016 / 10 / 25 (화) (1)

Berry curvature 유도

PRL 108, 196802 (2012) 논문 Eq. (3) 식으로부터

Eq. (4) Berry curvature 유도하는 것이 목표.

Eq. (3) : $\hat{H} = at\left(\tau k_x \hat{\sigma}_x + k_y \hat{\sigma}_y\right) + \frac{\Delta}{2}\hat{\sigma}_z - \lambda\tau\frac{\hat{\sigma}_z - 1}{2}\hat{S}_z.$

$$= \begin{pmatrix} \frac{\Delta}{2} & at\tau k_x - iatk_y & 0 & 0 \\ at\tau k_x + iatk_y & \frac{\Delta}{2} + \lambda\tau & 0 & 0 \\ 0 & 0 & \frac{\Delta}{2} & at\tau k_x - iatk_y \\ 0 & 0 & at\tau k_x + iatk_y & \frac{\Delta}{2} - \lambda\tau \end{pmatrix}.$$

with basis $\{ |d_{x^2-y^2}\uparrow\rangle, |d_{xy}\uparrow\rangle, |d_{x^2-y^2}\downarrow\rangle, |d_{xy}\downarrow\rangle \}$.

이 Hamiltonian 을 대각화 하면.

낮은 에너지 부터 $E_1 = \frac{1}{2}\left(\Delta - \lambda\tau - \sqrt{4a^2k_y^2t^2 + 4a^2k_x^2t^2\tau^2 + \lambda^2\tau^2}\right)$

$$E_2 = \frac{1}{2}\left(\Delta + \lambda\tau - \sqrt{4a^2k_y^2t^2 + 4a^2k_x^2t^2\tau^2 + \lambda^2\tau^2}\right)$$

$$E_3 = \frac{1}{2}\left(\Delta - \lambda\tau + \sqrt{4a^2k_y^2t^2 + 4a^2k_x^2t^2\tau^2 + \lambda^2\tau^2}\right)$$

$$E_4 = \frac{1}{2}\left(\Delta + \tau\lambda + \sqrt{4a^2k_y^2t^2 + 4a^2k_x^2t^2\tau^2 + \lambda^2\tau^2}\right).$$

$$|\psi_1\rangle = \left[\left(-\frac{i\left(\lambda\tau - \sqrt{4a^2k_y^2t^2 + 4a^2k_x^2t^2\tau^2 + \lambda^2\tau^2}\right)}{2at\,(k_y - ik_x\tau)}\right)|d_{x^2-y^2}\downarrow\rangle\right.$$

$$\left. + |d_{xy}\downarrow\rangle\right] / \text{norm.}$$

$$|\psi_2\rangle = \left[\left(\frac{i\left(\lambda\tau + \sqrt{4a^2k_y^2t^2 + 4a^2k_x^2t^2\tau^2 + \lambda^2\tau^2}\right)}{2at\,(k_y - ik_x\tau)}\right)|d_{x^2-y^2}\uparrow\rangle\right.$$

$$\left. + |d_{xy}\uparrow\rangle\right] / \text{norm}$$

$$|\psi_3\rangle = \left[\left(-\frac{i\left(\lambda\tau + \sqrt{4a^2k_y^2t^2 + 4a^2k_x^2t^2\tau^2 + \lambda^2\tau^2}\right)}{2at\,(k_y - ik_x\tau)}\right)|d_{x^2-y^2}\downarrow\rangle\right.$$

$$\left. + |d_{xy}\downarrow\rangle\right] / \text{norm}$$

$$|\psi_4\rangle = \left[\left(\frac{i\left(\lambda\tau - \sqrt{4a^2k_y^2t^2 + 4a^2k_x^2t^2\tau^2 + \lambda^2\tau^2}\right)}{2at\,(k_y - ik_x\tau)}\right|d_{x^2-y^2}\uparrow\rangle\right.$$

$$\left. + |d_{xy}\uparrow\rangle\right] / \text{norm.}$$

Berry curvature is defined by

$$\Omega_n(\vec{k}) = i\left(\langle \partial_{k_x} \psi_n(\vec{k}) \,|\, \partial_{k_y} \psi_n(\vec{k}) \rangle - \langle \partial_{k_y} \psi_n(\vec{k}) \,|\, \partial_{k_x} \psi_n(\vec{k}) \rangle \right)$$

n: band index.

Thus we have

$$\Omega_1(\vec{k}) = i\left(\langle \partial_{k_x} \psi_1(\vec{k}) \,|\, \partial_{k_y} \psi_1(\vec{k}) \rangle - \langle \partial_{k_y} \psi_1(\vec{k}) \,|\, \partial_{k_x} \psi_1(\vec{k}) \rangle \right)$$

$$= \frac{2a^2t^2\lambda\tau^2}{\left(\lambda^2\tau^2 + 4a^2t^2\left(k_y^2 + k_x^2\tau^2\right)\right)^{3/2}}.$$

$$\Omega_2(\vec{k}) = -\frac{2a^2t^2\lambda\tau^2}{\left(\lambda^2\tau^2 + 4a^2t^2\left(k_y^2 + k_x^2\tau^2\right)\right)^{3/2}}.$$

$$\Omega_3(\vec{k}) = -\frac{2a^2t^2\lambda\tau^2}{\left(\lambda^2\tau^2 + 4a^2t^2\left(k_y^2 + k_x^2\tau^2\right)\right)^{3/2}}.$$

$$\Omega_4(\vec{k}) = \frac{2a^2t^2\lambda\tau^2}{\left(\lambda^2\tau^2 + 4a^2t^2\left(k_y^2 + k_x^2\tau^2\right)\right)^{3/2}}$$