Effective Zeeman Term of Twisted Bilayer Graphene

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1 Without θ-dependence

We write the Hamiltonian as

$$H(\mathbf{k}) = \begin{pmatrix} \mathbf{k}\cdot\boldsymbol{\sigma} & T_1 & T_2 & T_3 \\ T_1 & (\mathbf{k}-\mathbf{q}_1)\cdot\boldsymbol{\sigma} & 0 & 0 \\ T_2 & 0 & (\mathbf{k}-\mathbf{q}_2)\cdot\boldsymbol{\sigma} & 0 \\ T_3 & 0 & 0 & (\mathbf{k}-\mathbf{q}_3)\cdot\boldsymbol{\sigma} \end{pmatrix}, \tag{1}$$

where

$$T_1 = w_0 + w_1\sigma_x, \qquad T_2 = w_0 + w_1\cos\frac{2\pi}{3}\sigma_x + w_1\sin\frac{2\pi}{3}\sigma_y, \qquad T_3 = w_0 + w_1\cos\frac{2\pi}{3}\sigma_x - w_1\sin\frac{2\pi}{3}\sigma_y, \tag{2}$$

$$\mathbf{q}_1 = (0,1), \qquad \mathbf{q}_2 = (-\frac{\sqrt{3}}{2}, -\frac{1}{2}), \qquad \mathbf{q}_3 = (\frac{\sqrt{3}}{2}, -\frac{1}{2}). \tag{3}$$

We assume an eigenstate with energy E has the form $\psi^T = (u_0, u_1, u_2, u_3)$. Then it satisfies

$$\mathbf{k}\cdot\boldsymbol{\sigma}u_0 + T_1u_1 + T_2u_2 + T_3u_3 = Eu_0, \tag{4}$$

$$T_iu_0 + (\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma}u_i = Eu_i, \qquad (i=1,2,3), \tag{5}$$

Using Eq. (5), we have

$$u_i = (E - (\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma})^{-1}T_iu_0 = \frac{E + (\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma}}{E^2 - (\mathbf{k}-\mathbf{q}_i)^2}T_iu_0. \tag{6}$$

Substituting this into Eq. (4), we have

$$\mathbf{k}\cdot\boldsymbol{\sigma}u_0 + \sum_{i=1}^{3} T_i\frac{E + (\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma}}{E^2 - (\mathbf{k}-\mathbf{q}_i)^2}T_iu_0 = Eu_0. \tag{7}$$

We find that the eigenenergies at $\mathbf{k}=0$ are

$$E_{1,2} - \sqrt{1+3w_0^2+3w_1^2}, \qquad E_3 = -1, \qquad E_{4,5} = 0, \qquad E_6 = 1, \qquad E_{7,8} = \sqrt{1+3w_0^2+3w_1^2}. \tag{8}$$

In the following, we focus on the zero-energy states. To solve the dispersion around $\mathbf{k}=0$, we linearize Eq. (7) as

$$\mathbf{k}\cdot\boldsymbol{\sigma}u_0 - \sum_{i=1}^{3} T_i(E + (\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma})T_i(1+2\mathbf{k}\cdot\mathbf{q}_i)u_0 = Eu_0. \tag{9}$$

Since

$$\sum_i T_i^2 = 3(w_0^2+w_1^2)\sigma_0, \qquad \sum_i T_i\sigma_{x,y}T_i = 3w_0^2\sigma_{x,y}, \tag{10}$$

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$$\sum_i T_i \mathbf{q}_i \cdot \boldsymbol{\sigma} T_i = 0, \qquad \sum_i 2\mathbf{k}\cdot\mathbf{q}_i T_i(-\mathbf{q}_i\cdot\boldsymbol{\sigma})T_i = -3(w_0^2 - w_1^2)\mathbf{k}\cdot\boldsymbol{\sigma} \tag{11}$$

we have

$$(1-3w_1^2)\mathbf{k}\cdot\boldsymbol{\sigma} u_0 = E(1+3w_0^2+3w_1^2)u_0. \tag{12}$$

Thus the dispersions of the zero-energy states are

$$E_4(\mathbf{k}) = -v|\mathbf{k}|, \qquad E_5(\mathbf{k}) = v|\mathbf{k}|, \qquad v = \frac{1-3w_1^2}{1+3w_0^2+3w_1^2}. \tag{13}$$

1.1 Eigenstates at magic-angle

At magic angle, we have $v=0$. We choose the eigenstates at $\mathbf{k}=0$ as C_3 eigenstates. To linear order of $\mathbf{k}$, the wavefunctions for the two zero-energy branches are

$$\psi_4(\mathbf{k}) \approx \frac{1}{\sqrt{N_4(\mathbf{k})}}\begin{pmatrix} u_- \\ -\frac{(\mathbf{k}-\mathbf{q}_1)\cdot\boldsymbol{\sigma}}{(\mathbf{k}-\mathbf{q}_1)^2}T_1u_- \\ -\frac{(\mathbf{k}-\mathbf{q}_2)\cdot\boldsymbol{\sigma}}{(\mathbf{k}-\mathbf{q}_2)^2}T_2u_- \\ -\frac{(\mathbf{k}-\mathbf{q}_3)\cdot\boldsymbol{\sigma}}{(\mathbf{k}-\mathbf{q}_3)^2}T_3u_- \end{pmatrix} \approx \frac{1}{\sqrt{N_4(\mathbf{k})}}\begin{pmatrix} u_- \\ -(\mathbf{k}-\mathbf{q}_1)\cdot\boldsymbol{\sigma}(1+2\mathbf{k}\cdot\mathbf{q}_1)T_1u_- \\ -(\mathbf{k}-\mathbf{q}_2)\cdot\boldsymbol{\sigma}(1+2\mathbf{k}\cdot\mathbf{q}_2)T_2u_- \\ -(\mathbf{k}-\mathbf{q}_3)\cdot\boldsymbol{\sigma}(1+2\mathbf{k}\cdot\mathbf{q}_3)T_3u_- \end{pmatrix}, \qquad u_- = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix}, \tag{14}$$

$$\psi_5(\mathbf{k}) \approx \frac{1}{\sqrt{N_5(\mathbf{k})}}\begin{pmatrix} u_+ \\ -\frac{(\mathbf{k}-\mathbf{q}_1)\cdot\boldsymbol{\sigma}}{(\mathbf{k}-\mathbf{q}_1)^2}T_1u_+ \\ -\frac{(\mathbf{k}-\mathbf{q}_2)\cdot\boldsymbol{\sigma}}{(\mathbf{k}-\mathbf{q}_2)^2}T_2u_+ \\ -\frac{(\mathbf{k}-\mathbf{q}_3)\cdot\boldsymbol{\sigma}}{(\mathbf{k}-\mathbf{q}_3)^2}T_3u_+ \end{pmatrix} \approx \frac{1}{\sqrt{N_4(\mathbf{k})}}\begin{pmatrix} u_- \\ -(\mathbf{k}-\mathbf{q}_1)\cdot\boldsymbol{\sigma}(1+2\mathbf{k}\cdot\mathbf{q}_1)T_1u_+ \\ -(\mathbf{k}-\mathbf{q}_2)\cdot\boldsymbol{\sigma}(1+2\mathbf{k}\cdot\mathbf{q}_2)T_2u_+ \\ -(\mathbf{k}-\mathbf{q}_3)\cdot\boldsymbol{\sigma}(1+2\mathbf{k}\cdot\mathbf{q}_3)T_3u_+ \end{pmatrix}, \qquad u_+ = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix}. \tag{15}$$

The normalization factors are

$$\begin{aligned} N_4(\mathbf{k}) \approx & 1 + \sum_i u_-^\dagger T_i \left(\frac{(\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma}}{(\mathbf{k}-\mathbf{q}_i)^2}\right)^2 T_i u_- \approx 1 + \sum_i u_-^\dagger T_i(1+2\mathbf{k}\cdot\mathbf{q}_i)T_iu_- \\ \approx & 1 + u_-^\dagger(3(w_0^2+w_1^2) + 6w_0w_1(k_y\sigma_x - k_x\sigma_y))u_- = 1+3(w_0^2+w_1^2), \end{aligned} \tag{16}$$

$$N_5(\mathbf{k}) \approx 1 + u_+^\dagger(3(w_0^2+w_1^2) + 6w_0w_1(k_y\sigma_x - k_x\sigma_y))u_+ = 1+3(w_0^2+w_1^2). \tag{17}$$

In the following, we will use ψ_4 and ψ_5 as bases for all calculations. We have assumed $v=0$ ($w_1 = \pm\frac{1}{\sqrt{3}}$) in the above calculations. When $v\neq 0$, $\psi_{4,5}$ are still correct at $\mathbf{k}=0$. However, at $\mathbf{k}\neq 0$, the energy eigenstates are linear combinations of them and higher energy bands. For simplicity, we will omit the contribution from higher energy bands. In other words, we always project the states into the bases $\psi_{4,5}$.

2 With θ-dependence

Now we consider the θ-dependent Hamiltonian:

$$\widetilde{H}(\mathbf{k}) = \begin{pmatrix} \mathbf{k}\cdot\boldsymbol{\sigma} & T_1 & T_2 & T_3 \\ T_1 & (\mathbf{k}-\mathbf{q}_1)\cdot\widetilde{\boldsymbol{\sigma}} & 0 & 0 \\ T_2 & 0 & (\mathbf{k}-\mathbf{q}_2)\cdot\widetilde{\boldsymbol{\sigma}} & 0 \\ T_3 & 0 & 0 & (\mathbf{k}-\mathbf{q}_3)\cdot\widetilde{\boldsymbol{\sigma}} \end{pmatrix}, \qquad \widetilde{\boldsymbol{\sigma}} = (\cos\theta\sigma_x + \sin\theta\sigma_y, -\sin\theta\sigma_x + \cos\theta\sigma_y). \tag{18}$$

To linear order of θ, we have

$$\begin{aligned} \Delta H(\mathbf{k}) = & H'(\mathbf{k}) - H(\mathbf{k}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \theta(\hat{z}\times(\mathbf{k}-\mathbf{q}_1))\cdot\boldsymbol{\sigma} & 0 & 0 \\ 0 & 0 & \theta(\hat{z}\times(\mathbf{k}-\mathbf{q}_2))\cdot\boldsymbol{\sigma}\cdot\boldsymbol{\sigma} & 0 \\ 0 & 0 & 0 & \theta(\hat{z}\times(\mathbf{k}-\mathbf{q}_3))\cdot\boldsymbol{\sigma} & 0 \end{pmatrix} \\ = & \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \theta(\mathbf{k}-\mathbf{q}_1)\times\boldsymbol{\sigma} & 0 & 0 \\ 0 & 0 & \theta(\mathbf{k}-\mathbf{q}_2)\times\boldsymbol{\sigma} & 0 \\ 0 & 0 & 0 & \theta(\mathbf{k}-\mathbf{q}_3)\times\boldsymbol{\sigma} & 0 \end{pmatrix}. \end{aligned} \tag{19}$$

2.1 Perturbation theory at magic-angle

The perturbed energies (to linear order of $\mathbf{k}$) are

$$\Delta E_4(\mathbf{k}) = \psi_4^\dagger(\mathbf{k})\Delta H(\mathbf{k})\psi_4(\mathbf{k}) = \frac{\theta}{1+3(w_0^2+w_1^2)}\sum_i (1+2\mathbf{k}\cdot\mathbf{q}_i)^2 u_-^\dagger T_i((\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma})((\mathbf{k}-\mathbf{q}_i)\times\boldsymbol{\sigma})((\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma})T_i u_-. \tag{20}$$

For any 2D vectors $\mathbf{q}, \mathbf{p}$, there is

$$(\mathbf{q}\times\boldsymbol{\sigma})(\mathbf{p}\cdot\boldsymbol{\sigma}) = (\mathbf{q}\times\mathbf{p})\sigma_0 - i\mathbf{q}\cdot\mathbf{p}\sigma_z, \qquad (\mathbf{q}\cdot\boldsymbol{\sigma})\cdot\sigma_z = -i\mathbf{q}\times\boldsymbol{\sigma}. \tag{21}$$

We have

$$\Delta E_4(\mathbf{k}) = \frac{\theta}{1+3(w_0^2+w_1^2)}\sum_i -u_-^\dagger T_i((\mathbf{k}-\mathbf{q}_i)\times\boldsymbol{\sigma})T_i u_-. \tag{22}$$

According to

$$\sum_i T_i \mathbf{q}_i \times \boldsymbol{\sigma} T_i = -6w_0 w_1 \sigma_0 \tag{23}$$

and Eq. (10), we have

$$\Delta E_4(\mathbf{k}) = -\frac{\theta}{1+3(w_0^2+w_1^2)} u_-^\dagger(3w_0^2\mathbf{k}\cdot\boldsymbol{\sigma} - 6w_0w_1\sigma_0)T_i u_- = \frac{6w_0w_1\theta}{1+3(w_0^2+w_1^2)}. \tag{24}$$

Similarly, we have

$$\Delta E_5(\mathbf{k}) = -\frac{\theta}{1+3(w_0^2+w_1^2)} u_+^\dagger(3w_0^2\mathbf{k}\cdot\boldsymbol{\sigma} - 6w_0w_1\sigma_0)T_i u_+ = \frac{6w_0w_1\theta}{1+3(w_0^2+w_1^2)}. \tag{25}$$

Thus the perturbation does not split the two bands.

Similar to Eqs. (14) and (15), we can write the eigenstates as (to linear terms of θ, $\mathbf{k}$)

$$\begin{aligned}
\widetilde{\psi}_4(\mathbf{k}) \approx & \frac{1}{\sqrt{\widetilde{N}_4(\mathbf{k})}}\begin{pmatrix} u_- \\ \frac{\Delta E + (\mathbf{k}-\mathbf{q}_1)\cdot\widetilde{\boldsymbol{\sigma}}}{\Delta E^2 - (\mathbf{k}-\mathbf{q}_1)^2} T_1 u_- \\ \frac{\Delta E + (\mathbf{k}-\mathbf{q}_2)\cdot\widetilde{\boldsymbol{\sigma}}}{\Delta E^2 - (\mathbf{k}-\mathbf{q}_2)^2} T_2 u_- \\ \frac{\Delta E + (\mathbf{k}-\mathbf{q}_3)\cdot\widetilde{\boldsymbol{\sigma}}}{\Delta E^2 - (\mathbf{k}-\mathbf{q}_3)^2} T_3 u_- \end{pmatrix} \\
\approx & \frac{1}{\sqrt{\widetilde{N}_4(\mathbf{k})}}\begin{pmatrix} u_- \\ -(\Delta E + (\mathbf{k}-\mathbf{q}_1)\cdot\boldsymbol{\sigma} + \theta(\mathbf{k}-\mathbf{q}_1)\times\boldsymbol{\sigma})(1+2\mathbf{k}\cdot\mathbf{q}_1)T_1 u_- \\ -(\Delta E + (\mathbf{k}-\mathbf{q}_2)\cdot\boldsymbol{\sigma} + \theta(\mathbf{k}-\mathbf{q}_2)\times\boldsymbol{\sigma})(1+2\mathbf{k}\cdot\mathbf{q}_2)T_2 u_- \\ -(\Delta E + (\mathbf{k}-\mathbf{q}_3)\cdot\boldsymbol{\sigma} + \theta(\mathbf{k}-\mathbf{q}_3)\times\boldsymbol{\sigma})(1+2\mathbf{k}\cdot\mathbf{q}_3)T_3 u_- \end{pmatrix},
\end{aligned} \tag{26}$$

$$\widetilde{\psi}_5(\mathbf{k}) \approx \frac{1}{\sqrt{\widetilde{N}_5(\mathbf{k})}}\begin{pmatrix} u_+ \\ -(\Delta E + (\mathbf{k}-\mathbf{q}_1)\cdot\boldsymbol{\sigma} + \theta(\mathbf{k}-\mathbf{q}_1)\times\boldsymbol{\sigma})(1+2\mathbf{k}\cdot\mathbf{q}_1)T_1 u_+ \\ -(\Delta E + (\mathbf{k}-\mathbf{q}_2)\cdot\boldsymbol{\sigma} + \theta(\mathbf{k}-\mathbf{q}_2)\times\boldsymbol{\sigma})(1+2\mathbf{k}\cdot\mathbf{q}_2)T_2 u_+ \\ -(\Delta E + (\mathbf{k}-\mathbf{q}_3)\cdot\boldsymbol{\sigma} + \theta(\mathbf{k}-\mathbf{q}_3)\times\boldsymbol{\sigma})(1+2\mathbf{k}\cdot\mathbf{q}_3)T_3 u_+ \end{pmatrix}. \tag{27}$$

The normalization factors are

$$\begin{aligned}
\widetilde{N}_4(\mathbf{k}) \approx & N_4(\mathbf{k}) + \sum_i (1+2\mathbf{k}\cdot\mathbf{q}_i)^2 u_-^\dagger \left(T_i(\Delta E + \theta(\mathbf{k}-\mathbf{q}_1)\times\boldsymbol{\sigma})(\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma}T_i + h.c.\right) u_- \\
\approx & N_4(\mathbf{k}) + \sum_i (1+4\mathbf{k}\cdot\mathbf{q}_i) u_-^\dagger \left(T_i(\Delta E(\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma} - i\theta|\mathbf{k}-\mathbf{q}_i|^2\sigma_z)T_i + h.c.\right) u_- \\
\approx & N_4(\mathbf{k}) + 2\sum_i (1+4\mathbf{k}\cdot\mathbf{q}_i) u_-^\dagger \left(T_i \Delta E(\mathbf{k}-\mathbf{q}_i)\cdot\boldsymbol{\sigma}T_i\right) u_- \\
\approx & N_4(\mathbf{k}) \approx 1+3(w_0^2+w_1^2).
\end{aligned} \tag{28}$$

In the last step we have used Eqs. (10) and (11) and $u_-^+\sigma_{x,y}u_- = 0$. Similarly, we have

$$\widetilde{N}_5(\mathbf{k}) \approx N_5(\mathbf{k}) \approx 1+3(w_0^2+w_1^2). \tag{29}$$

We find the orbital magnetizations of ψ_4 and ψ_5 are

$$
\begin{aligned}
L_4 = & - L_5 = -\frac{i}{2}\sum_{ij}\epsilon_{ij}\langle\partial_{k_i}\psi_4(\mathbf{k})|\widetilde{H}(\mathbf{k}) - \Delta E_4(\mathbf{k})|\partial_{k_j}\psi_4(\mathbf{k})\rangle_{\mathbf{k}=0} = \frac{3\Delta E(w_0^2 - w_1^2)}{N_4(0)} \\
= & \frac{18 w_0 w_1 (w_0^2 - w_1^2)\theta}{(1 + 3(w_0^2 + w_1^2))^2}.
\end{aligned}
\tag{30}
$$