# 1 Theory

In the model introduced by Liu *et al.*, only the orbitals of the M atom are included. We denote the wave functions of the three orbitals of the M atom as

$$|\phi_1\rangle = |d_{z^2}\rangle\,, \quad |\phi_2\rangle = |d_{xy}\rangle\,, \quad |\phi_3\rangle = |d_{x^2-y^2}\rangle\,. \tag{1}$$

The Bloch wavefunction in this model has the form

$$\psi^{\lambda}_{\mathbf{k}}(\mathbf{r}) = \sum_{j=1}^{3} C^{\lambda}_{j}(\mathbf{k}) \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \phi_j(\mathbf{r}-\mathbf{R}). \tag{2}$$

The coefficents $C^{\lambda}_{j}(\mathbf{k})$ are the solutions of the eigenvalue equation

$$\sum_{jj'}^{3} \left[H^{\mathrm{TB}}_{jj'}(\mathbf{k}) - \varepsilon_\lambda(\mathbf{k}) S_{jj'}(\mathbf{k})\right] C^{\lambda}_{j}(\mathbf{k}) = 0, \tag{3}$$

where

$$H^{\mathrm{TB}}_{jj'}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_j(\mathbf{r})\right| H_{1\mathrm{e}} \left|\phi_{j'}(\mathbf{r}-\mathbf{R})\right\rangle, \tag{4}$$

and

$$S_{jj'}(\mathbf{k}) = \sum_{\mathbf{R}} \left\langle \phi_j(\mathbf{r}) \middle| \phi_{j'}(\mathbf{r}-\mathbf{R})\right\rangle \approx \delta_{jj'}. \tag{5}$$

In the case $B \neq 0$, wave function can be expressed as the coefficients of $C^{\lambda}_{ji}$ in the tight-binding wave function

$$\psi_{\lambda,\mathbf{k}}(\mathbf{r}) = \sum_{j}^{3} \sum_{i}^{2q} C^{\lambda}_{ji}(\mathbf{k}) \sum_{\alpha}^{N_{\mathrm{UC}}} e^{i\mathbf{k}\cdot(\mathbf{R}_\alpha+\mathbf{r}_i)} \phi_j(\mathbf{r}-\mathbf{R}_\alpha-\mathbf{r}_i). \tag{6}$$

where $j = 1, 2, 3$ and $i = 1...2q$. We have shown that, under an uniform magnetic field, Bloch bands $\lambda$ construct Landau levels at small fields and become fractal-structured at strong fields, which is known as the Hofstadter butterfly.

We now consider a new basis consisting of three eigenfunctions of the angular momentum operators $L^2$ and $L_z$, for $l = 2, m = 0, \pm 2$,

$$\left|\tilde{\phi}_1\right\rangle = |d_{m=0}\rangle\,, \quad \left|\tilde{\phi}_2\right\rangle = |d_{m=+2}\rangle\,, \quad \left|\tilde{\phi}_3\right\rangle = |d_{m=-2}\rangle\,. \tag{7}$$

The new basis can be obtained from the old one by the transformation

$$\left|\tilde{\phi}_j\right\rangle = \sum_{j'} W_{j'j} \left|\phi_j\right\rangle, \tag{8}$$

where

$$W = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{9}$$

In particular,

$$\left|\tilde{\phi}_1\right\rangle = \left|\phi_1\right\rangle, \tag{10}$$

$$\left|\tilde{\phi}_2\right\rangle = \frac{i}{\sqrt{2}}\left|\phi_2\right\rangle + \frac{1}{\sqrt{2}}\left|\phi_3\right\rangle, \tag{11}$$

$$\left|\tilde{\phi}_3\right\rangle = -\frac{i}{\sqrt{2}}\left|\phi_2\right\rangle + \frac{1}{\sqrt{2}}\left|\phi_3\right\rangle. \tag{12}$$

The TB Hamiltonian in new basis reads

$$\tilde{H}^{\mathrm{TB}}(\mathbf{k}) = W^{\dagger} H^{\mathrm{TB}}(\mathbf{k}) W, \tag{13}$$

where $H^{\mathrm{TB}} = H^{\mathrm{NN}}$ or $H^{\mathrm{TNN}}$.

Tại $p = 1$, $q = 4723$, tần số cyclotron được tính theo công thức

$$\begin{aligned} \hbar\omega_c &= E_{n+1} - E_n \\ \Rightarrow \omega_c &= \frac{E_{n+1} - E_n}{\hbar}, \end{aligned} \tag{14}$$

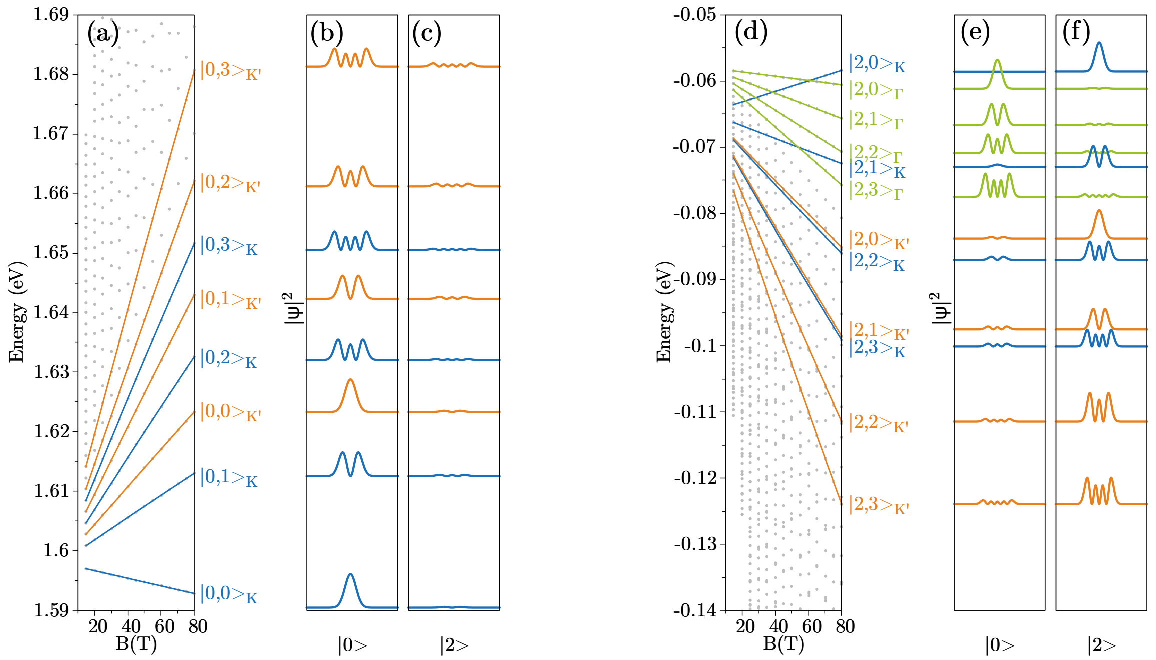
và khối lượng hiệu dụng cyclotrong được tính bằng công thức

$$\omega_c = \frac{eB}{m^*} \Rightarrow m^* = \frac{eB}{\omega_c} = \frac{eB}{\frac{E_{n+1}-E_n}{\hbar}} = \frac{eB\hbar}{E_{n+1} - E_n} \tag{15}$$

trong đó $n$ là chỉ số mức Landau. Hàm sóng của 2 mức Landau kế tiếp nhau ở điểm $K$ được thể hiện qua Fig.3. Ở hình 3(a),(b),(c) là hàm sóng ở mức Landau $n = 1$, với dải $2q + 4$, hình 3(d),(e),(f) là hàm sóng ở mức Landau $n = 2$ với dải $2q + 8$

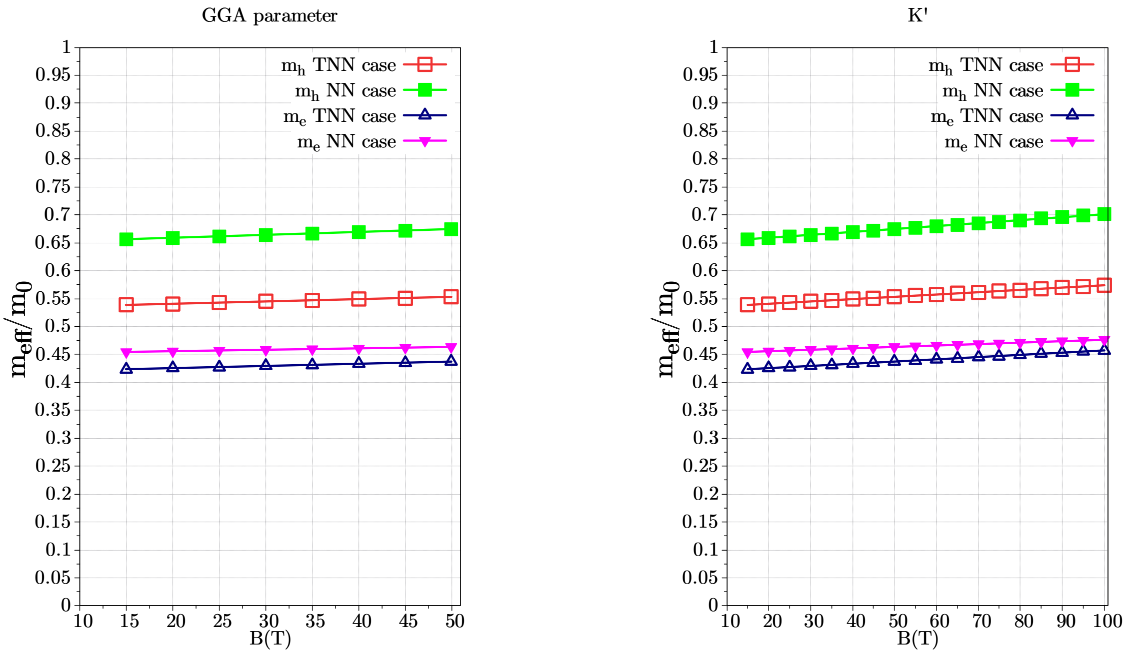
## 1.1 Effective mass

### Monolayer $MoS_2$



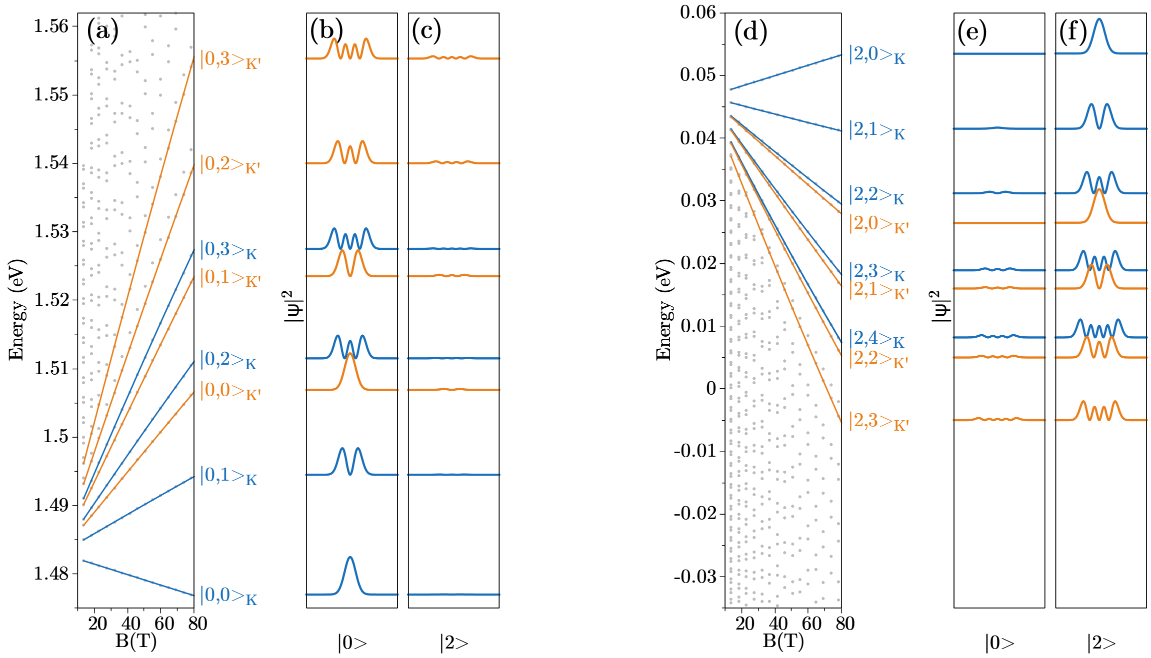

Hình 1: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng cho $MoS_2$



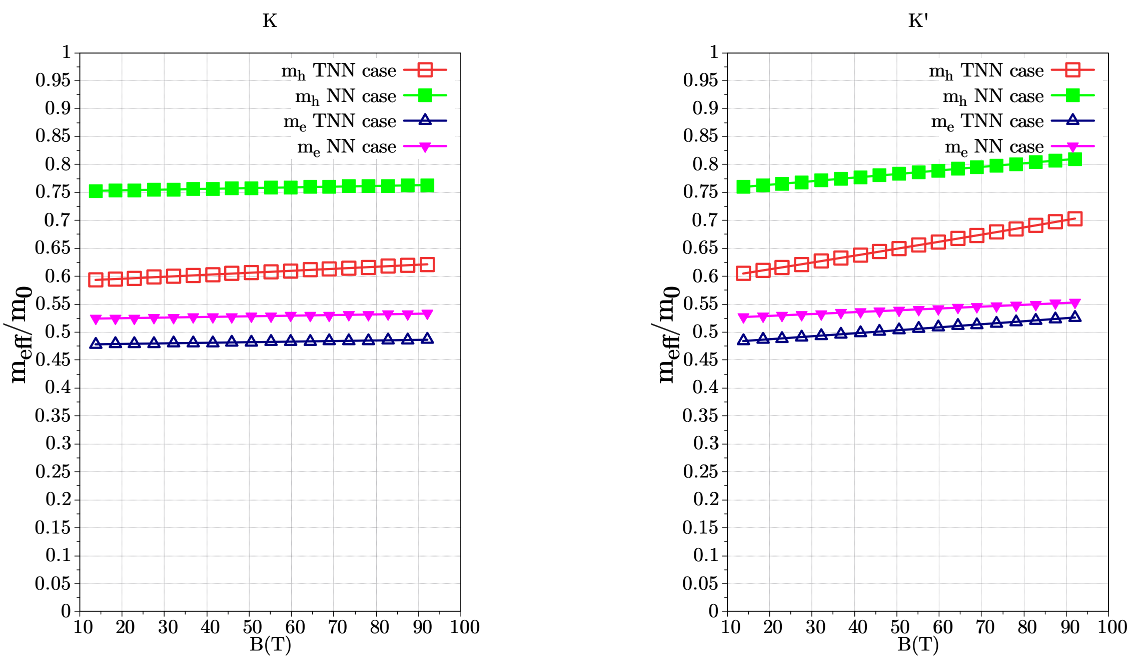

Hình 2: Khối lượng hiệu dụng.

**Monolayer $MoSe_2$**



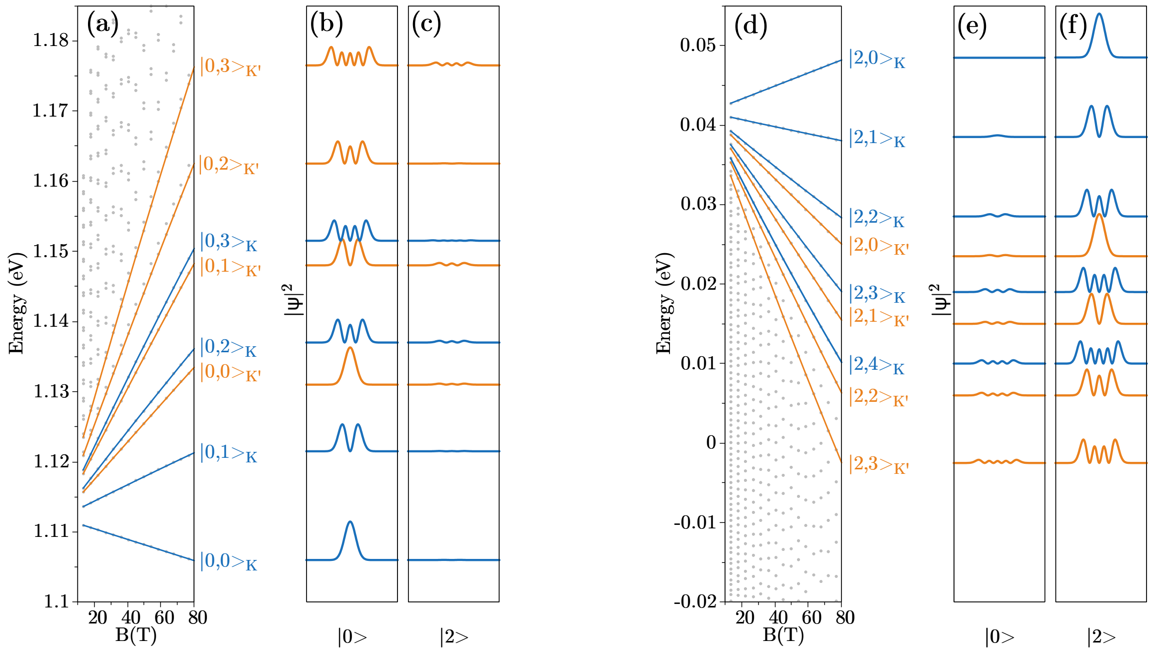

Hình 3: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng



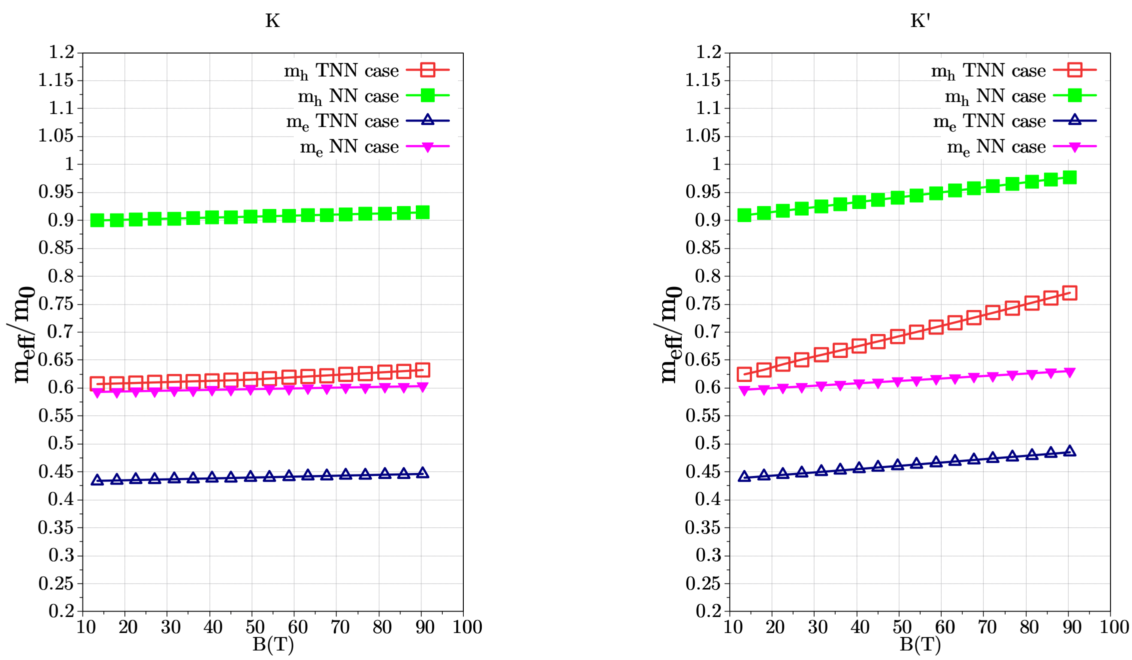

Hình 4: Khối lượng hiệu dụng.

## Monolayer $MoTe_2$




Hình 5: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng




Hình 6: Khối lượng hiệu dụng.

**Monolayer $WS_2$**