

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

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

The Bloch wavefunction in this model has the form

$$\psi_{\mathbf{k}}^\lambda(\mathbf{r}) = \sum_{j=1}^3 C_j^\lambda(\mathbf{k}) \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \phi_j(\mathbf{r} - \mathbf{R}). \quad (2)$$

The coefficients $C_j^\lambda(\mathbf{k})$ are the solutions of the eigenvalue equation

$$\sum_{jj'}^3 \left[H_{jj'}^{\text{TB}}(\mathbf{k}) - \varepsilon_\lambda(\mathbf{k}) S_{jj'}(\mathbf{k}) \right] C_j^\lambda(\mathbf{k}) = 0, \quad (3)$$

where

$$H_{jj'}^{\text{TB}}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi_j(\mathbf{r}) | H_{1e} | \phi_{j'}(\mathbf{r} - \mathbf{R}) \rangle, \quad (4)$$

and

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

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

$$\psi_{\lambda,\mathbf{k}}(\mathbf{r}) = \sum_j^3 \sum_i^{2q} C_{ji}^\lambda(\mathbf{k}) \sum_{\alpha}^{N_{\text{UC}}} e^{i\mathbf{k}\cdot(\mathbf{R}_\alpha + \mathbf{r}_i)} \phi_j(\mathbf{r} - \mathbf{R}_\alpha - \mathbf{r}_i). \quad (6)$$

where $j = 1, 2, 3$ and $i = 1 \dots 2q$. We have shown that, under an uniform magnetic field, Bloch bands λ 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 $l = 2, m = 0, \pm 2$,

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

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

$$|\tilde{\phi}_j\rangle = \sum_{j'} W_{j'j} |\phi_j\rangle, \quad (8)$$

where

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

In particular,

$$|\tilde{\phi}_1\rangle = |\phi_1\rangle, \quad (10)$$

$$|\tilde{\phi}_2\rangle = \frac{i}{\sqrt{2}} |\phi_2\rangle + \frac{1}{\sqrt{2}} |\phi_3\rangle, \quad (11)$$

$$|\tilde{\phi}_3\rangle = -\frac{i}{\sqrt{2}} |\phi_2\rangle + \frac{1}{\sqrt{2}} |\phi_3\rangle. \quad (12)$$

The TB Hamiltonian in new basis reads

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

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

The cyclotron frequency can be obtained from the energy difference between two Landau levels

$$\hbar\omega_c = E_{n+1} - E_n, \quad (14)$$

which gives

$$\omega_c = \frac{E_{n+1} - E_n}{\hbar}. \quad (15)$$

On the other hand, the cyclotron frequency is also defined as

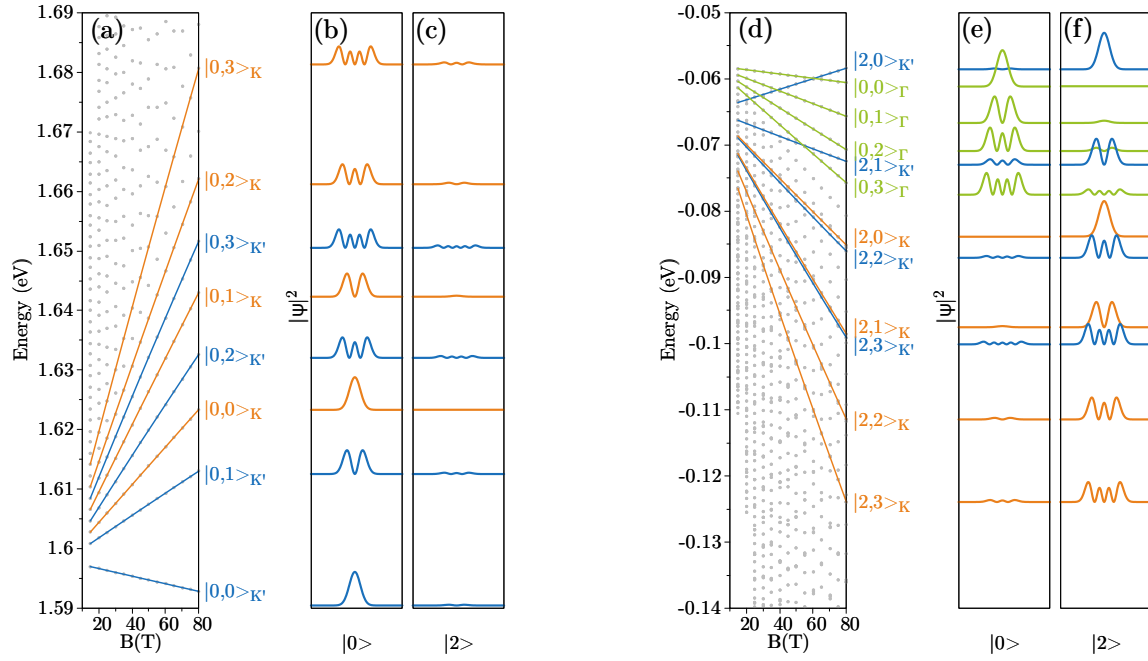
$$\omega_c = \frac{eB}{m^*}. \quad (16)$$

Combining the two expressions, the effective mas can be written as

$$m^* = \frac{eB}{\omega_c} = \frac{eB}{\frac{E_{n+1}-E_n}{\hbar}} = \frac{eB\hbar}{E_{n+1} - E_n}. \quad (17)$$

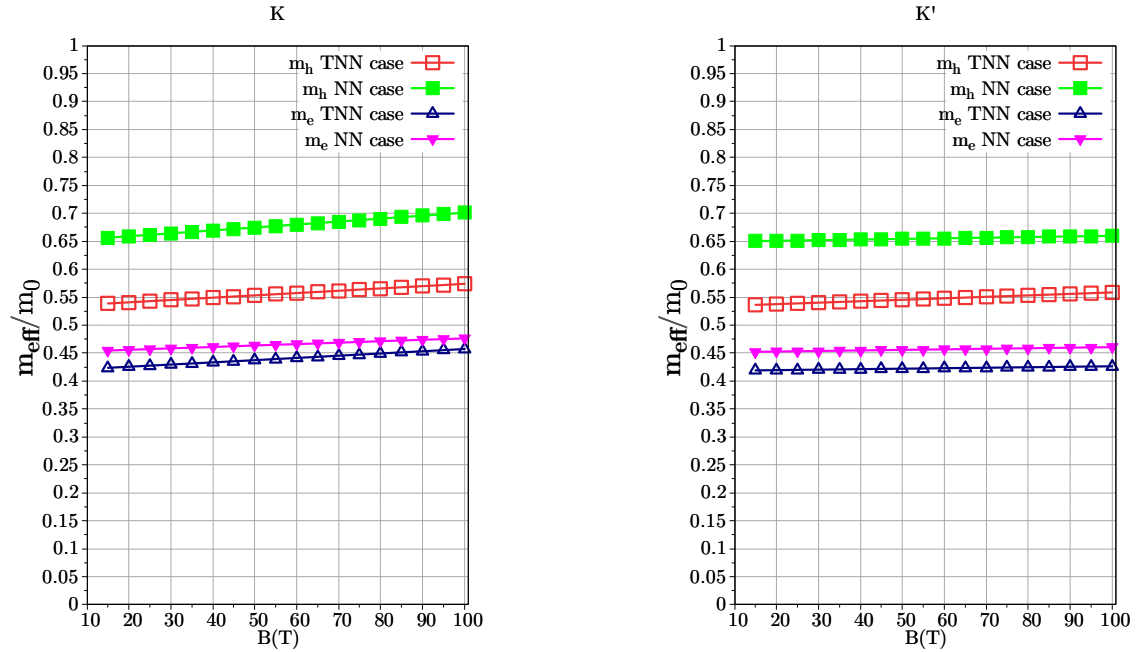
1.1 Effective mass

Monolayer MoS₂



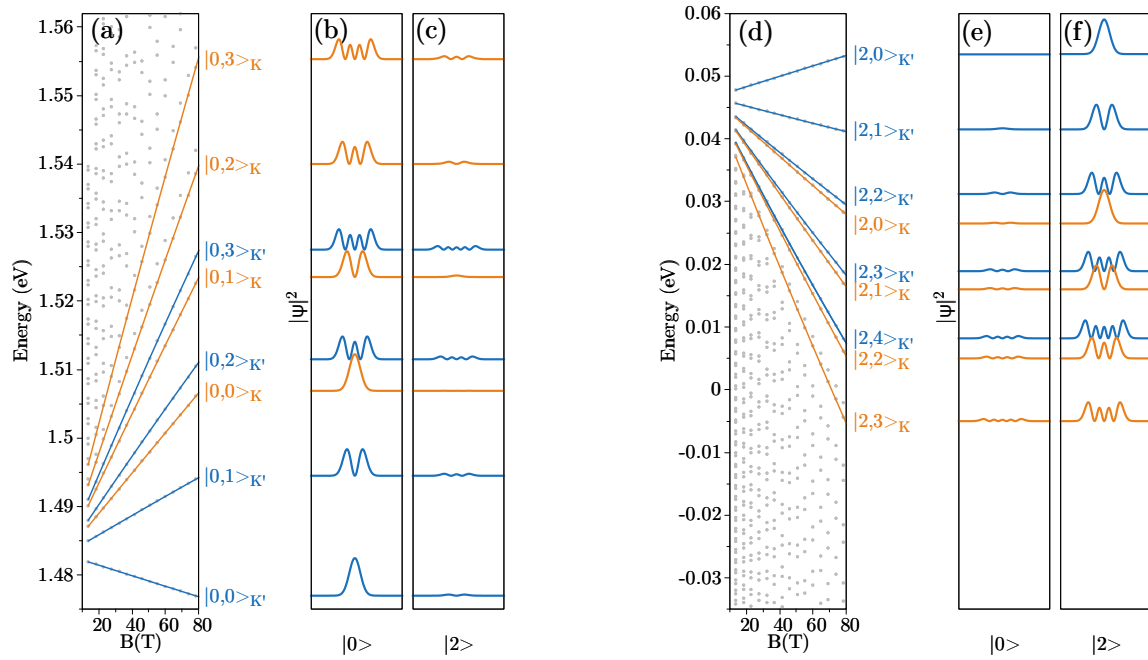
Hình 1: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng cho MoS₂



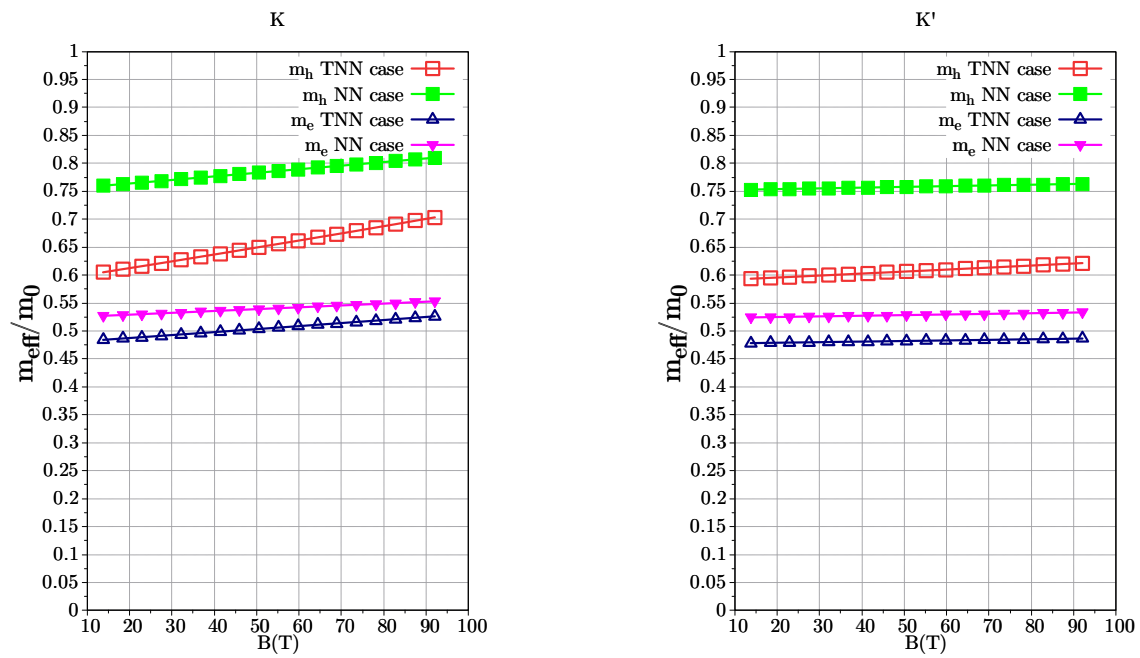
Hình 2: Khối lượng hiệu dụng.

Monolayer MoSe₂



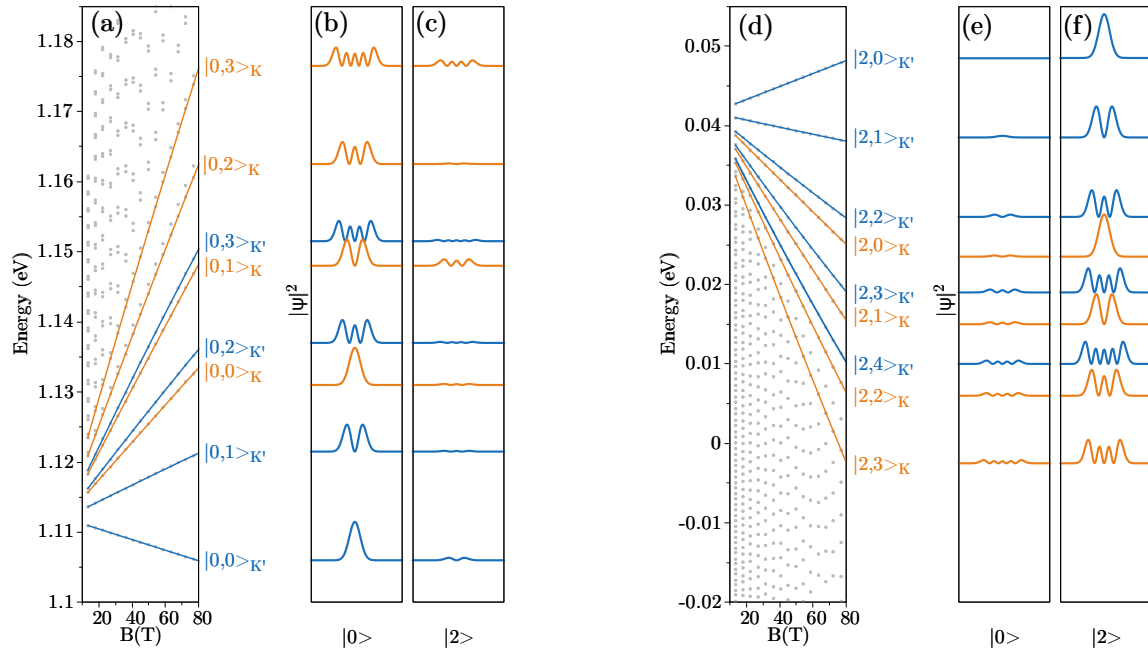
Hình 3: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng



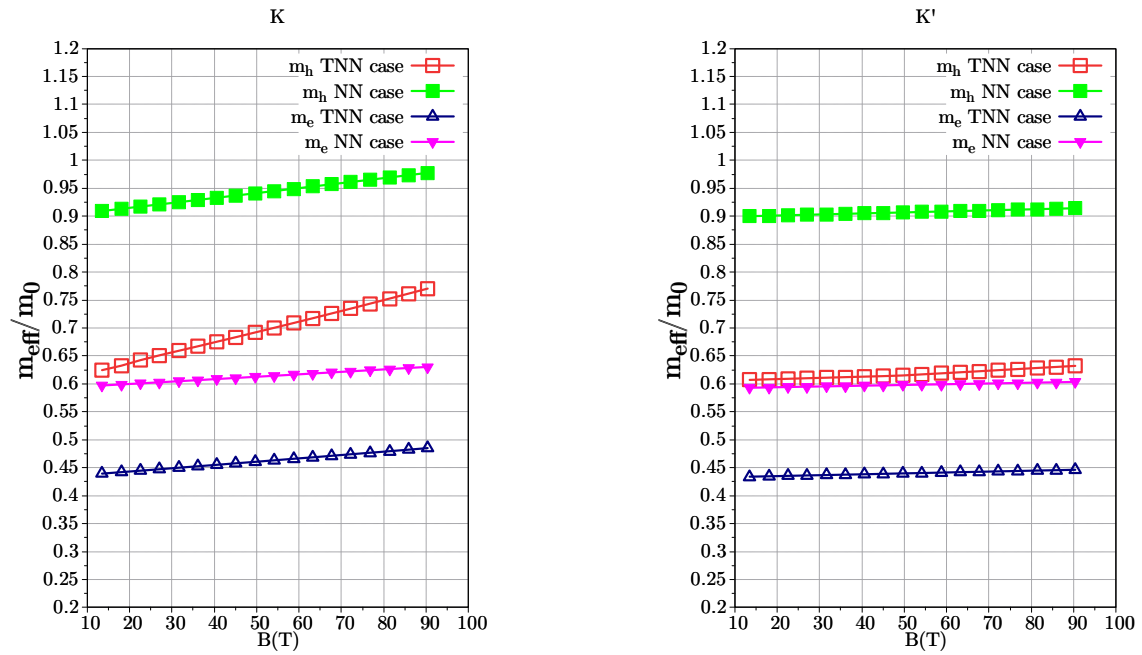
Hình 4: Khối lượng hiệu dụng.

Monolayer MoTe₂



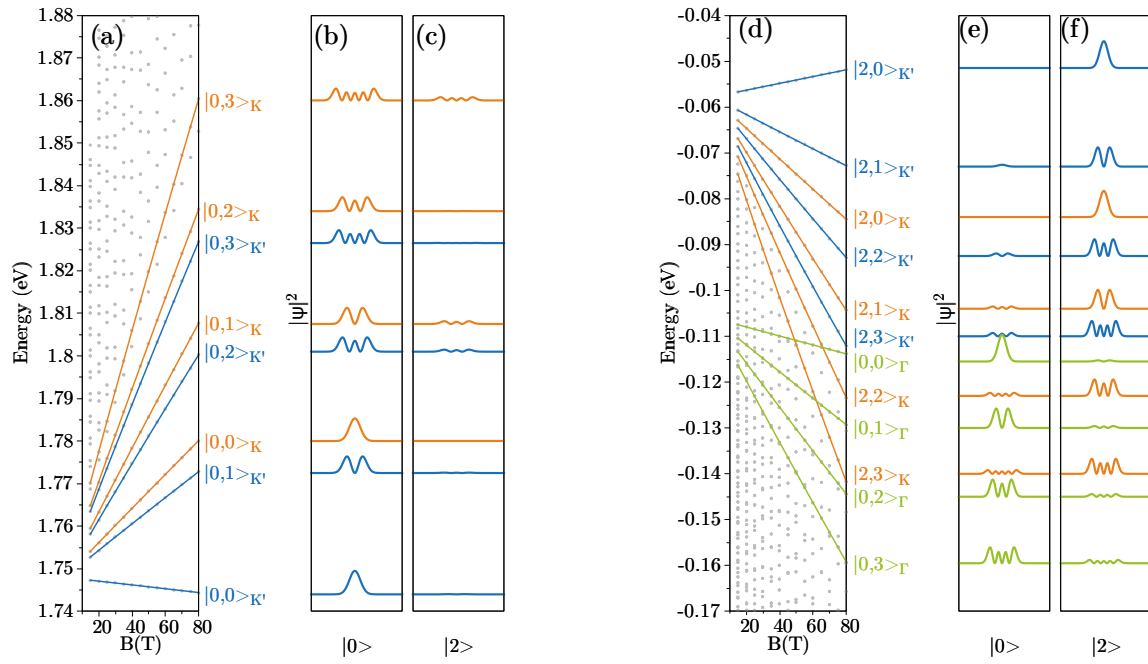
Hình 5: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng



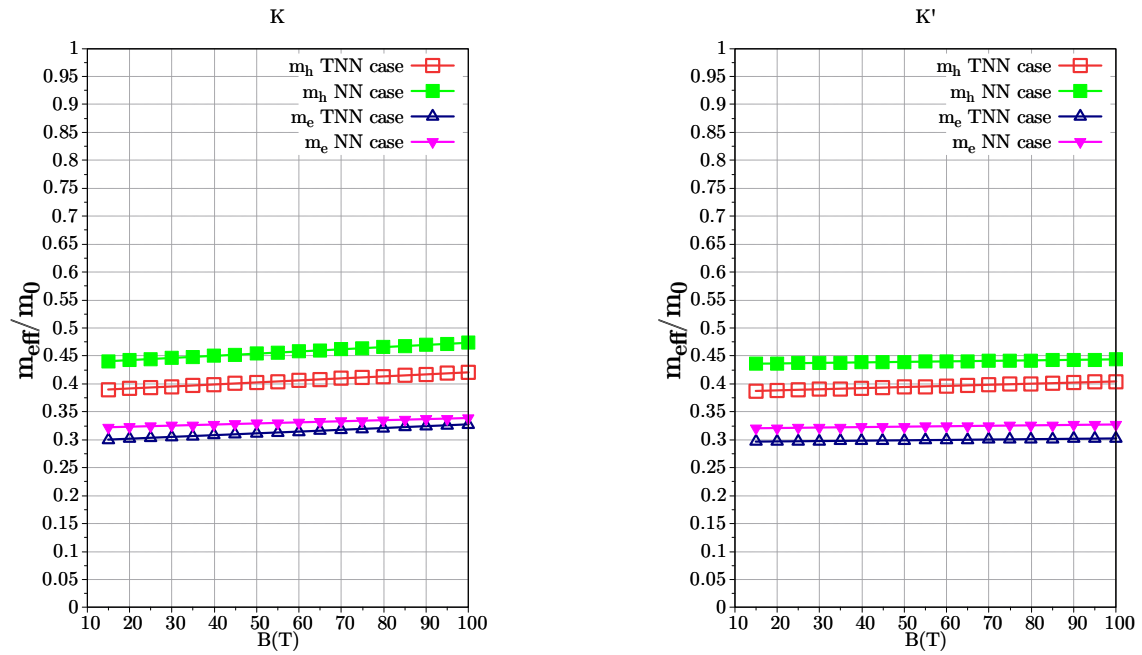
Hình 6: Khối lượng hiệu dụng.

Monolayer WS₂



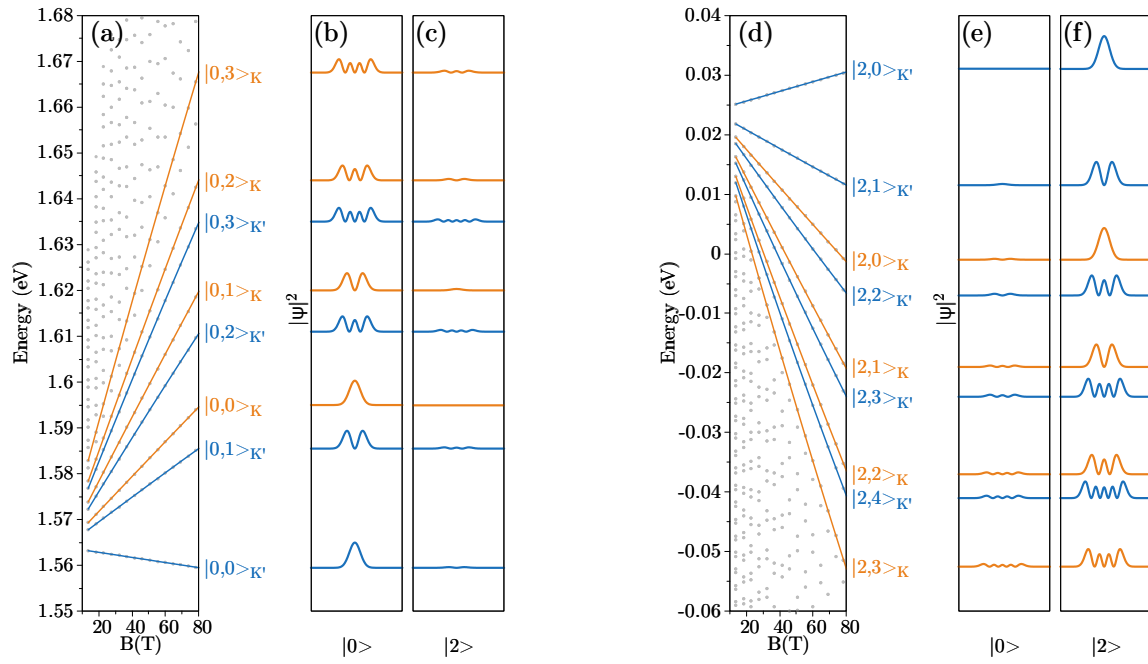
Hình 7: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng



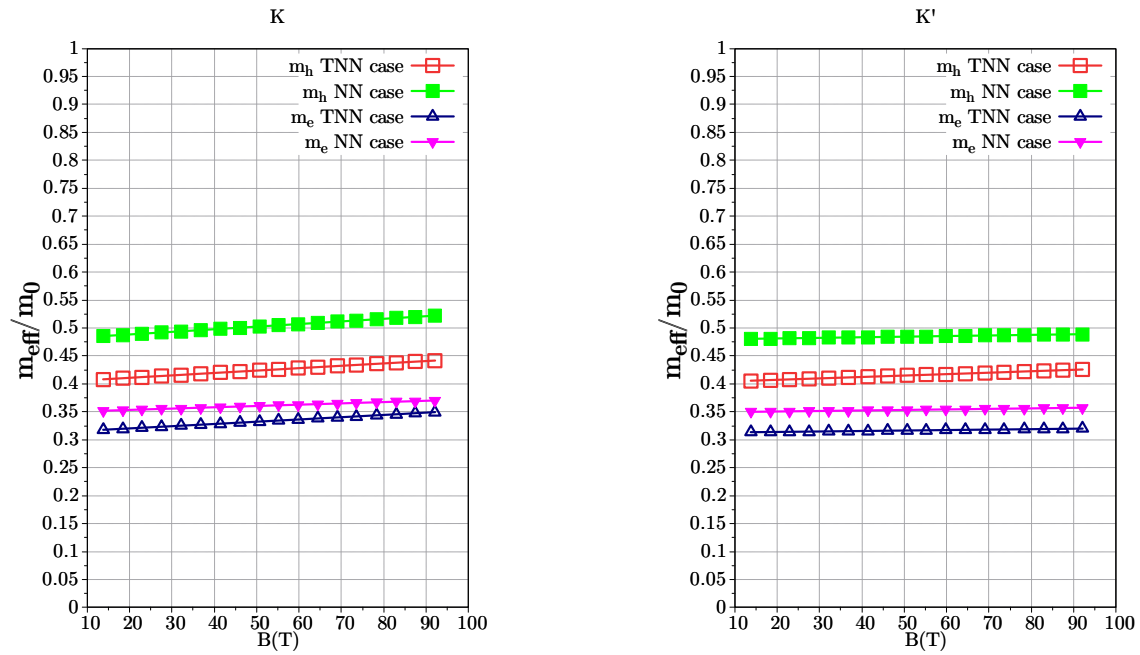
Hình 8: Khối lượng hiệu dụng.

Monolayer WSe₂



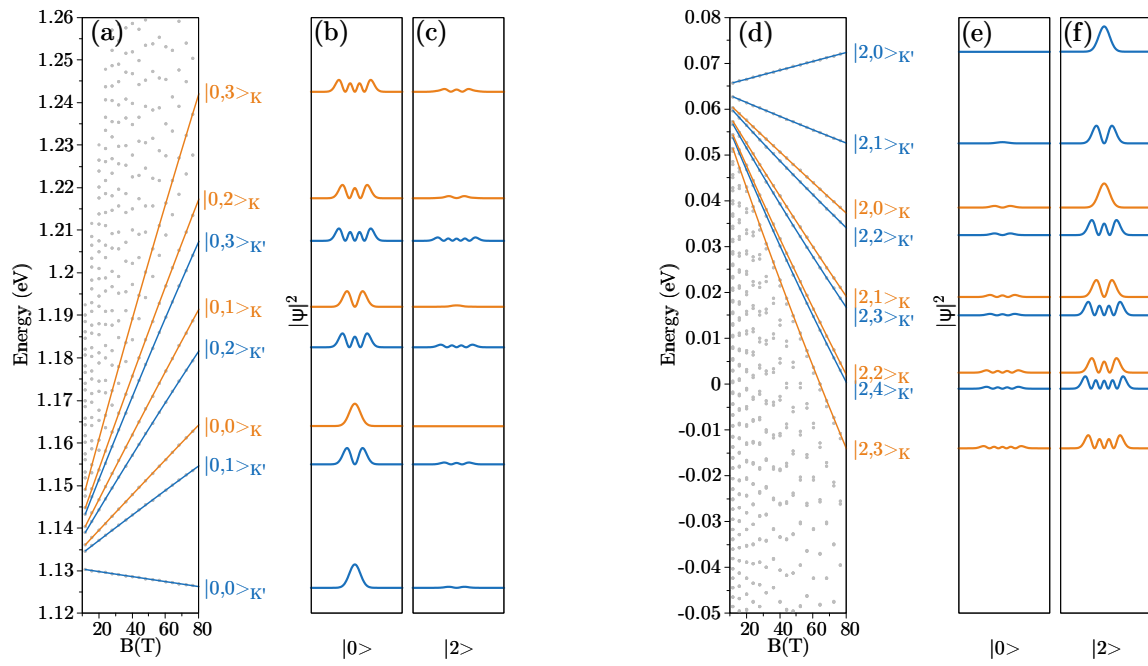
Hình 9: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng



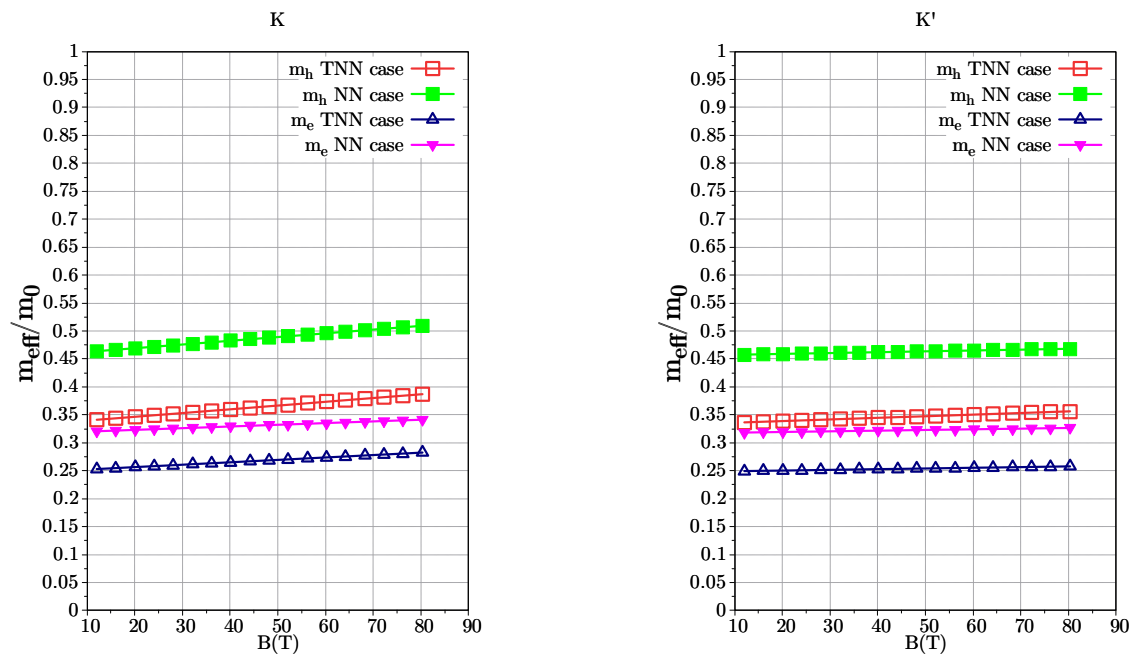
Hình 10: Khối lượng hiệu dụng.

Monolayer WTe₂



Hình 11: Hàm sóng của 2 mức Landau kế tiếp nhau.

Khối lượng hiệu dụng



Hình 12: Khối lượng hiệu dụng.