TFY4245/FY8917 Solid State Physics, Advanced Course

Problemset 2

NTNU

Institutt for fysikk

SUGGESTED SOLUTION

Problem 1

The problem text states that the band is parabolic, i.e. $E = \hbar^2 k^2/2m_{\text{eff}}$ where m_{eff} is the effective mass. By reading out the energy at a certain k-value, we can then compute the ratio of the effective mass and the bare electron mass m_e:

$$\frac{m_{\text{eff}}}{m_e} = \frac{\hbar^2 k^2}{2m_e E}. \tag{1}$$

From the figure in the problem text, consider first curve A. We see that $E = 0.07$ eV at $k = 0.1$ Å^{-1}. Using that 1 eV $= 1.602 \times 10^{-19}$ J and 1 Å = 10^{-10} m, we obtain

$$\frac{m_{\text{eff}}^{\text{A}}}{m_e} \simeq 0.54. \tag{2}$$

For curve B, the energy is ten times higher at the same k-point. Thus, we conclude that

$$\frac{m_{\text{eff}}^{\text{A}}}{m_e} \simeq 0.05. \tag{3}$$

In general, the flatter the band, the higher the effective electron mass. This also enhances the density of states at a given k-point.

Problem 2

(a) We obtain

$$\begin{aligned}
\langle i|\alpha(\boldsymbol{n}\times\boldsymbol{\sigma})\cdot\hat{\boldsymbol{p}}|j\rangle &= \alpha(\boldsymbol{n}\times\boldsymbol{\sigma})\cdot\langle i|\hat{\boldsymbol{p}}|j\rangle \\
&= \alpha(\boldsymbol{n}\times\boldsymbol{\sigma})\int d\boldsymbol{r}\int d\boldsymbol{r}'\langle i|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\hat{\boldsymbol{p}}|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|j\rangle \\
&= \alpha(\boldsymbol{n}\times\boldsymbol{\sigma})\int d\boldsymbol{r}\int d\boldsymbol{r}'\phi_i^*(\boldsymbol{r})\hat{\boldsymbol{p}}(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}')\phi_j(\boldsymbol{r}') \\
&= \alpha(\boldsymbol{n}\times\boldsymbol{\sigma})\int d\boldsymbol{r}\phi_i^*(\boldsymbol{r})\hat{\boldsymbol{p}}(\boldsymbol{r})\phi_j(\boldsymbol{r}).
\end{aligned} \tag{4}$$

Here, $\hat{\boldsymbol{p}}(\boldsymbol{r}) = -\imath\nabla_{\boldsymbol{r}}$ and $\phi_i(\boldsymbol{r})$ is the Wannier wavefunctions in real space.

(b) We obtain (writing simply $\hat{\boldsymbol{p}}$ from now on)

$$\begin{aligned}
-i\alpha\int d\boldsymbol{r}\phi_i^*(\boldsymbol{r})\hat{\boldsymbol{p}}\phi_j(\boldsymbol{r}) &= -i\alpha\sum_m\hat{\boldsymbol{m}}\int d\boldsymbol{r}\phi_i^*(\boldsymbol{r})\frac{1}{2}[\phi_{j+\hat{\boldsymbol{m}}}(\boldsymbol{r})-\phi_{j-\hat{\boldsymbol{m}}}(\boldsymbol{r})] \\
&= -\frac{i\alpha}{2}\sum_m\hat{\boldsymbol{m}}(\delta_{i,j+\hat{\boldsymbol{m}}}-\delta_{i,j-\hat{\boldsymbol{m}}}) \\
&= \frac{i\alpha}{2}\sum_m\hat{\boldsymbol{m}}(\delta_{i,j-\hat{\boldsymbol{m}}}-\delta_{i,j+\hat{\boldsymbol{m}}}).
\end{aligned} \tag{5}$$

Here, the summation over m is over the spatial components of $\boldsymbol{p}$, i.e. $m \in \{x,y,z\}$.

(c) We have found that

$$\langle i\alpha|\hat{h}|j\beta\rangle = \frac{i}{2}\alpha\sum_m(\boldsymbol{n}\times\boldsymbol{\sigma})_m(\delta_{i,j-\hat{\boldsymbol{m}}}-\delta_{i,j+\hat{\boldsymbol{m}}}). \tag{6}$$

Writing out the summation gives

$$\begin{aligned}\langle i\alpha|\hat{h}|j\beta\rangle &= \frac{i}{2}\alpha(\boldsymbol{n}\times\boldsymbol{\sigma})\cdot\sum_m[\hat{\boldsymbol{m}}(\delta_{i,j-\hat{\boldsymbol{m}}}-\delta_{i,j+\hat{\boldsymbol{m}}}) \\ &= \frac{i}{2}\alpha(\boldsymbol{n}\times\boldsymbol{\sigma})\cdot\boldsymbol{d}_{ij}. \end{aligned}\tag{7}$$

Now use that $(\boldsymbol{n}\times\boldsymbol{\sigma})\cdot\boldsymbol{d}_{ij} = \boldsymbol{n}\cdot(\boldsymbol{\sigma}\times\boldsymbol{d}_{ij})$ and arrive at

$$H = \frac{i}{2}\alpha\sum_{ij\alpha\beta}\boldsymbol{n}\cdot(\boldsymbol{\sigma}\times\boldsymbol{d}_{ij})_{\alpha\beta}c^\dagger_{i\alpha}c_{j\beta} \tag{8}$$

where the summation over ij is only for nearest-neighbors.

(d) If inversion symmetry is broken, the terms in the Hamiltonian should not be invariant under an exchange $i \leftrightarrow j$ since that would be the outcome of a parity operation. Since $\boldsymbol{d}_{ij} = -\boldsymbol{d}_{ji}$, we see that the antisymmetric spin-orbit interaction indeed breaks inversion symmetry. Had we Fourier-transformed the spin-orbit interaction to momentum space, the resulting Hamiltonian terms would not have been invariant under $\boldsymbol{k} \to -\boldsymbol{k}$.