TFY4245/FY8917 Solid State Physics, Advanced Course

Problemset 2

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Problem 1

Figure 1 shows the parabolic E versus k relationship in the conduction band for an electron in two particular semiconductor materials A and B. Determine the effective mass (in units of the free electron mass m) of the two electrons.

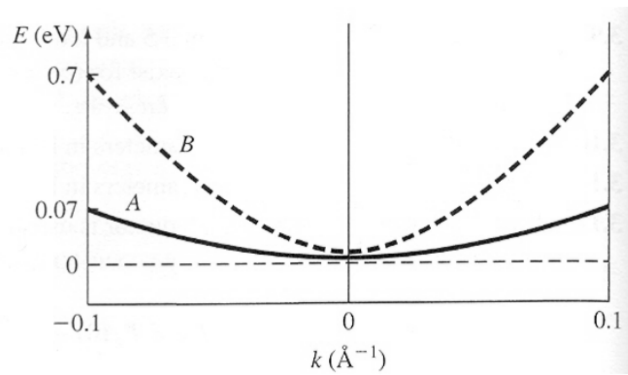

Figure 1: Energy-momentum dispersion for electron conduction band in two particular semiconductor materials A and B. Figure taken from `https://ocw.tudelft.nl/wp-content/uploads/SSP_E1_ex609.pdf`.

Problem 2

Inversion symmetry breaking is an important effect occuring in many situations in condensed matter physics. One distinguishes between structural and bulk inversion asymmetry. Structural inversion asymmetry arises due to the geometry of a given setup, such as at the interface between two materials or at the surface of a thin film. Bulk inversion asymmetry arises when the crystal structure itself lacks a center of inversion.

In the presence of such inversion asymmetry, a so-called antisymmetric spin-orbit potential arises. The most famous example of this is Rashba spin-orbit coupling. Asymmetric spin-orbit interactions such as Rashba-coupling exists because of both inversion asymmetry in the potential and atomic spin-orbit interactions. A simple picture accounting for this is that the inversion asymmetric potential produces an effective local electric field from $\boldsymbol{E} = -\nabla V(\boldsymbol{r})$. An electron moving in this field will then have its spin couple to this electric field because the electron spin effectively sees a moving electric field from its reference frame, which induces a magnetic field in its reference frame (from the special theory of relativity, we know that an observer in a frame moving relative a frame with a stationary electric field will observe a magnetic field in addition to an electric field in their frame).

The Rashba spin-orbit interaction Hamilton operator $\hat{h}$ can in first quantization be written as

$$\hat{h} = \alpha(\boldsymbol{n} \times \hat{\boldsymbol{S}}) \cdot \hat{\boldsymbol{p}} \tag{1}$$

Here, α is the magnitude of the Rashba spin-orbit interaction, $\hat{\boldsymbol{p}}$ is the momentum operator, $\hat{\boldsymbol{S}}$ is the electron spin operator, and $\boldsymbol{n}$ is a unit vector along the direction that breaks inversion symmetry. For a thin-film in the xy-plane, $\boldsymbol{n}$ would thus point in the $\boldsymbol{z}$-direction.

Note that one can use the cyclic property of the triple product to rewrite the above $\hat{h}$ as a Zeeman-coupling between a spin and a momentum-dependent effective magnetic field $\boldsymbol{B}(\hat{\boldsymbol{p}})$.

In this problem, we will derive the second quantized expression for the spin-orbit interaction operator in terms of the operators $c_{i\sigma}, c_{i\sigma}^{\dagger}$ which annihilate and create a fermion of spin σ on lattice site i in a Wannier state. In other words, we want to write the Hamiltonian as

$$H = \sum_{ij\alpha\beta} \langle i\alpha|h|j\beta\rangle c_{i\alpha}^{\dagger} c_{j\beta}. \tag{2}$$

The task is to find an expression for the matrix element $\langle i\alpha|\hat{h}|j\beta\rangle$.

Consider the spin part first. We know that spin states $|\alpha\rangle$ can be represented as spinors and the spin operator $\hat{\boldsymbol{S}}$ as a matrix in such a way that $\langle\alpha|\hat{\boldsymbol{S}}|\beta\rangle = \boldsymbol{\sigma}_{\alpha\beta}$ where $\boldsymbol{\sigma}$ is the Pauli matrix vector. What remains is to carry out the orbital (spatial) part of the expectation value.

(a) Insert two completeness relations for a set of position operator eigenstates, $\int d\boldsymbol{r}|\boldsymbol{r}\rangle\langle\boldsymbol{r}| = 1$, and show that

$$\langle i|\alpha(\boldsymbol{n} \times \boldsymbol{\sigma}) \cdot \hat{\boldsymbol{p}}|j\rangle = \alpha(\boldsymbol{n} \times \boldsymbol{\sigma}) \int d\boldsymbol{r} \phi_i^*(\boldsymbol{r}) \hat{\boldsymbol{p}} \phi_j^*(\boldsymbol{r}). \tag{3}$$

What are the functions $\phi_i(\boldsymbol{r})$?

(b) We thus need to evaluate the integral

$$-i \int d\boldsymbol{r} \phi_i^*(\boldsymbol{r}) \alpha \partial_m \phi_j(\boldsymbol{r}) \tag{4}$$

where $m = \{x, y, z\}$. The derivative can be discretized on a lattice:

$$\partial_m \phi_j(\boldsymbol{r}) = \frac{\phi_{j+\hat{\boldsymbol{m}}}(\boldsymbol{r}) - \phi_{j-\hat{\boldsymbol{m}}}(\boldsymbol{r})}{2} \tag{5}$$

where $\phi_{j\pm\hat{\boldsymbol{m}}}(\boldsymbol{r}) = \phi(\boldsymbol{r} - \boldsymbol{R}_j \pm \hat{\boldsymbol{m}})$ and $\boldsymbol{R}_j$ is the position of lattice site j and $\hat{\boldsymbol{m}}$ is a unit vector in the $\boldsymbol{m}$ direction. If we assume that ϕ_j is highly localized around position $\boldsymbol{R}_j$, the overlap between the probability distributions of atoms at neighboring lattice sites is small, allowing us to write:

$$\int d\boldsymbol{r} \phi_i^*(\boldsymbol{r}) \phi_j(\boldsymbol{r}) = \delta_{ij} \tag{6}$$

Use the above considerations to show that

$$\int d\boldsymbol{r} \phi_i^*(\boldsymbol{r}) \alpha \hat{p}_m \phi_j(\boldsymbol{r}) = \frac{i}{2} \alpha (\delta_{i,j-\hat{\boldsymbol{m}}} - \delta_{i,j+\hat{\boldsymbol{m}}}). \tag{7}$$

(c) To make the notation a bit more compact, define the vector $\boldsymbol{d}_{ij}$ connecting sites i and j:

$$\boldsymbol{d}_{ij} = \sum_m \hat{\boldsymbol{m}}(\delta_{i,j-\hat{\boldsymbol{m}}} - \delta_{i,j+\hat{\boldsymbol{m}}}). \tag{8}$$

For instance, if $i = i_0$ and $j = i_0 + \hat{\boldsymbol{x}}$, we verify that we get the correct answer $\boldsymbol{d}_{ij} = \hat{\boldsymbol{x}}$.

Use the definition of the $\boldsymbol{d}$-vector above to show that the final second quantized form of the Rashba spin-orbit interaction operator is

$$H = \frac{i}{2} \sum_{ij\alpha\beta} \alpha c^\dagger_{i\alpha} \hat{\boldsymbol{n}} \cdot (\boldsymbol{\sigma} \times \boldsymbol{d}_{ij})_{\alpha\beta} c_{j\beta}. \tag{9}$$

where the sum over ij is restricted to nearest neighbors and $\alpha, \beta = \uparrow, \downarrow = \pm 1$.

(d) The Rashba spin-orbit interaction was argued to arise from atomic spin-orbit coupling and the lack of inversion symmetry. How is the lack of inversion symmetry in the system manifested mathematically in the final form for the second-quantized Hamiltonian?