1. Spin-orbit coupling in a 2DEG. Consider electrons confined to a “quantum well,” which is modeled by hard walls at $z = 0$ and $z = d$ (i.e. infinite potential for $z < 0$ and $z > d$, and zero potential elsewhere – like a particle in a box). Except for the hard wall potential, the electrons are free and have mass $m$.

(a) Show that the energy eigenstates for a single electron of arbitrary spin have the form

$$\psi_{k,p}(r) = A \begin{pmatrix} \beta_\uparrow \\ \beta_\downarrow \end{pmatrix} \sin \left( \frac{\pi p z}{d} \right) e^{i \mathbf{k} \cdot \mathbf{r}_\perp},$$

where $\mathbf{k} = (k_x, k_y)$ is the in-plane wavevector, $\mathbf{r}_\perp = (x, y)$, $p = 1, 2, 3, \ldots$, and $A$ is a normalization coefficient (don’t bother to find $A$). Because spin will play an important role starting in part (c), we explicitly write the electron wavefunction as a two-component spinor, and $\beta_\uparrow$ and $\beta_\downarrow$ are the spin-up and spin-down components. Find the corresponding energies $E_p(k)$. The different “bands” labeled by $p$ are called subbands.

(b) Suppose we fill this band structure with a two-dimensional density of electrons $n$ – that is, in this problem, $n$ is the number of electrons per unit area. There is a special value of the density $n^*$ so that, for $n < n^*$, only the lowest subband is occupied. Find $n^*$. From now on we shall assume $n < n^*$, in which case we can really think about this system as a two-dimensional electron gas (2DEG).

(c) We shall include a particular kind of spin-orbit coupling called a “Rashba” term. This comes from the microscopic form of the spin orbit coupling $H_{SO} = \lambda \mathbf{\sigma} \cdot (\mathbf{k} \times \nabla V)$, where $V = -e\phi$ is the electrostatic potential energy. Here, $\mathbf{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ is a vector of the three Pauli matrices acting on the spinor components of the wavefunction, and $\mathbf{k}$ is the electron’s wavevector. Now suppose there is an electric field pointing in the $z$-direction – there generally will be such a field when the quantum well is not perfectly symmetric. In this case it can be shown (you don’t have to show it!) that this leads to a correction to the energy of the lowest subband, which is the Rashba term:

$$H_R = \alpha (k_y \sigma^x - k_x \sigma^y).$$

For simplicity, assume $\alpha > 0$. Ignoring constant terms, the Hamiltonian for an electron of given $\mathbf{k}$ in the lowest subband is then

$$H = \frac{\hbar^2 k^2}{2m} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \alpha (k_y \sigma^x - k_x \sigma^y).$$

The Rashba term lifts the twofold spin degeneracy of the lowest subband, splitting it into two bands with energies $\epsilon_{\pm}(k)$. Calculate and plot $\epsilon_{\pm}(k)$. You should find that there is a critical density $n_c$, so that for $n < n_c$ only the lower band is occupied, but for $n > n_c$ both bands are occupied. Find $n_c$. For both $n < n_c$ and $n > n_c$, describe the shape of the Fermi surface in each band.

For reference, the Pauli matrices are

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
(d) We denote a state in the lower or upper band by $|\psi_{k,\pm}\rangle$. Each occupied state gives the following contribution to the total spin density:

$$S_{\pm}(k) = \hbar \langle \psi_{k,\pm} | \sigma^{z} | \psi_{k,\pm} \rangle. \quad (7)$$

Calculate $S_{\pm}(k)$. Note that in order to calculate this, you will need to find the eigenvectors of the Hamiltonian in Eq. (3). As a function of the density $n$, what is the total spin density of the ground state?

(e) Imagine an electric field $\mathbf{E} = (E_x, E_y)$ is applied in the plane of the quantum well. Assuming $n > n_c$, show that a spin density is induced by this applied electric field, and calculate the induced spin density. To do this treat both upper and lower bands using the Boltzmann equation in the relaxation time approximation – you will need to write down two Boltzmann equations, one for each band. For simplicity, assume both bands are governed by the same relaxation time $\tau$. Solve the Boltzmann equations to linear order in $\mathbf{E}$. Using these solutions, and $S_{\pm}(k)$ from part (d), calculate the total spin density to linear order in $\mathbf{E}$. Express your answer in terms of the density $n$ and other given parameters.

2. **Stoner mean-field theory of ferromagnetism.** In this problem, we shall apply the Hartree-Fock approximation to an electron gas with short-range repulsive interactions, and explore the possibility of a ferromagnetic ground state. Consider the Hamiltonian $\hat{H} = H_{\text{Kin}} + H_{\text{int}}$, where

$$H_{\text{Kin}} = \int d^3r \psi_\sigma^\dagger(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 \right] \psi_\sigma(r), \quad (8)$$

and

$$H_{\text{int}} = U \int d^3r \, \psi_\sigma^\dagger(r) \psi_\sigma(r) \psi_\sigma^\dagger(r) \psi_\sigma(r). \quad (9)$$

Here $\psi_\sigma^\dagger(r)$ is the usual creation operator for an electron at $r$ with spin $\sigma$, there is an implicit sum over repeated spin indices, and we consider repulsive interactions ($U > 0$). The total number of electrons is fixed to be $N$, and the volume is $V$, so the density is $n = N/V$.

Remember that in the Hartree-Fock approximation, we want to find a Slater determinant wavefunction $|\psi_{SD}\rangle$ that minimizes the variational energy $E_{\text{var}} = \langle \psi_{SD}|H|\psi_{SD}\rangle$. Ferromagnetic ground states contain different numbers of up- and down-spin electrons. Therefore we define:

$$\langle \psi_{SD}|\psi_\uparrow^\dagger(r)\psi_\uparrow(r)|\psi_{SD}\rangle = n_\uparrow \quad (10)$$

$$\langle \psi_{SD}|\psi_\downarrow^\dagger(r)\psi_\downarrow(r)|\psi_{SD}\rangle = n_\downarrow, \quad (11)$$

where $n_\uparrow$ and $n_\downarrow$ are the densities of spin-up and spin-down electrons, respectively – we assume that they do not vary in space. These add up to the total density $n = n_\uparrow + n_\downarrow$. We still assume that “off-diagonal” expectation values vanish, that is

$$\langle \psi_{SD}|\psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r')|\psi_{SD}\rangle = 0. \quad (12)$$

This is equivalent to assuming that the magnetization of the ferromagnet is polarized in the $z$-direction.

(a) Apply the Hartree-Fock approximation to find an expression for $E_{\text{var}}$ in terms of $n_\uparrow$ and $n_\downarrow$. For a given value of $U$, explain how to use the expression for $E_{\text{var}}$ to determine whether the ground state is ferromagnetic. Explain how to determine the spin density $S^z = (n_\uparrow - n_\downarrow)/2$ of the ground state.

(b) Show that, as a function of $U$, there are three regimes of ground state behavior. You should find the following three regimes: First, for $U < U_{c1}$, the ground state is nonmagnetic (i.e. $S^z = 0$). Second, for $U_{c1} < U < U_{c2}$, the ground state is ferromagnetic but is not fully polarized, meaning that $S^z$ does not attain its maximum value of $\pm n/2$. Finally, for $U > U_{c2}$, the ground state is fully polarized, with $S^z = \pm n/2$. Find $U_{c1}$ and $U_{c2}$ in terms of $n$, $m$ and $\hbar$. You should give exact expressions for $U_{c1}$ and $U_{c2}$ – that is, don’t solve for them numerically.

3. Ashcroft + Mermin 12.4, but do part (c) as (slightly) modified below.

Modified part (c): Assume that $R_1 = -1/n_c e c$ and $R_2 = 1/n_h e c$, as appropriate for a free-electron-like electron band and hole band, respectively. In this case, deduce directly from (12.73) the form (12.55) of the high-field Hall coefficient. Discuss the limiting high-field behavior in the case $n_{\text{eff}} = 0$ (i.e. for a compensated two-band metal). Show that in this case the magneto-resistance increases as $H^2$ with increasing field.
4. Magnetic field in tight-binding models.

(a) Begin with the tight-binding model on the two-dimensional square lattice,

$$ H = -t \sum_{\mathbf{R}} \left[ (c^\dagger_{\mathbf{R}\sigma} c_{\mathbf{R}+\mathbf{a}_x,\sigma} + c^\dagger_{\mathbf{R}+\mathbf{a}_x,\sigma} c_{\mathbf{R}\sigma}) + (c^\dagger_{\mathbf{R}\sigma} c_{\mathbf{R}+\mathbf{a}_y,\sigma} + c^\dagger_{\mathbf{R}+\mathbf{a}_y,\sigma} c_{\mathbf{R}\sigma}) \right]. $$  \hfill (13)

Here lattice sites are labeled by the Bravais lattice vector $\mathbf{R} = a(n_x \mathbf{x} + n_y \mathbf{y})$ for integer $n_x$ and $n_y$, and a sum over the repeated spin index $\sigma$ is implied. The operator $c^\dagger_{\mathbf{R}\sigma}$ creates an electron at the site $\mathbf{R}$ with spin $\sigma$, and

$$ \{ c_{\mathbf{R}\sigma}, c^\dagger_{\mathbf{R}'\sigma'} \} = 0 \quad \text{and} \quad \{ c_{\mathbf{R}\sigma}, c^\dagger_{\mathbf{R}'\sigma'} \} = \delta_{\sigma\sigma'} \delta_{\mathbf{R}\mathbf{R}'}. $$  \hfill (14)

Solve for the band structure of this tight binding model, giving your result in terms of the energy $\epsilon(\mathbf{k})$, where $\mathbf{k}$ is the crystal momentum. For half-filling (i.e. one electron per lattice site, on average), draw the Fermi surface.

(b) Imagine that a spatially constant magnetic field is turned on, pointing perpendicular to the plane of the square lattice (i.e. in the $z$-direction). Ignore the Zeeman coupling of the magnetic field to the electron spin. Write down (but do not try to solve!) a modified tight-binding Hamiltonian that accounts for the coupling of the electrons to the magnetic field. It is easiest to express the modified Hamiltonian in terms of the vector potential $\mathbf{A}$. Rather than resorting to detailed calculation, justify your result using simple physical arguments.

Hint 1: The Hamiltonian needs to be gauge-invariant. This means that it should be invariant under $\mathbf{A} \to \mathbf{A} + \nabla \lambda$ ($\mathbf{A}$ is the vector potential, and $\lambda$ is an arbitrary scalar function of position), together with an appropriate rotation of the phase of the electron creation and annihilation operators.

Hint 2: Try thinking in terms of the Aharonov-Bohm effect, which says that if an electron moves in a closed loop encircling a magnetic flux $\Phi$, its wavefunction picks up a phase factor $e^{2\pi i \Phi/\Phi_0}$, where $\Phi_0 = hc/e$. In order to think along these lines, you may want to think about each term of the Hamiltonian as a “hopping” process, that takes an electron from one site and moves it to a neighboring one.

Hint 3: The Hamiltonian you need to write down does not involve adding any extra terms to Eq. (13), but rather involves modifying the coefficients of the terms already present. This does not leave a lot of freedom for different kinds of modifications.

(c) Suppose a field is applied so that exactly $\Phi = hc/2e$ magnetic flux passes through each face of the square lattice. Solve for the tight-binding band structure in this case. (Hint: you will need to work with a unit cell containing two sites, but using more than two sites is not necessary. In order to get the Hamiltonian into a tractable form, you may need to make a partial gauge-transformation, where you make a gauge transformation of the vector potential, but don’t do anything to the electron creation and annihilation operators. It is okay to do this, because such partial gauge transformations can be achieved by making a unitary transformation, which does not affect the energy spectrum.) At half-filling, describe the Fermi surface, if there is one.