Magnetic oscillations in silicene

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Abstract

In this work the magnetic oscillations (MO) in pristine silicene at $T = 0$ K are studied. Considering a constant electron density we obtain analytical expressions for the ground state internal energy and magnetization, under a perpendicular electric and magnetic field, taking in consideration the Zeeman effect. It is found that the MO are sawtooth-like, depending on the change in the last occupied energy level. This leads us to a classification of the MO peaks in terms of the Landau level (LL), valley or spin changes. Using this classification we analyze the MO for different values of the electric field $E_z$. When $E_z = 0$, the energy levels have a valley degeneracy and the MO peaks occur only whenever the last energy level changes its LL and/or spin. When $E_z \neq 0$, the valley degeneracy is broken and new MO peaks appear, associated with the valley change in the last energy level. By analyzing the MO peaks amplitude it is possible to extract information about the Fermi velocity and the spin-orbit interaction strength. Finally we analyze the MO frequencies, which can also be associated with the change of LL, valley or spin in the last energy level.

1. Introduction

In the past few years silicene has been gaining considerable interest in the scientific community \cite{1,2,3}. Like graphene, silicene has a 2D hexagonal structure with silicon atoms at each lattice site, with two interpenetrating sublattices $A$ and $B$. The reciprocal space is also a hexagonal lattice in the momentum space, which in turn defines the Brillouin zone. Silicene is best described with a tight binding (TB) model, which leads to an effective Dirac-like Hamiltonian in the low energy approximation, with the sublattices $A$ and $B$ acting as a pseudospin degree of freedom \cite{4,6,6}. Nevertheless, silicon distinguish itself from graphene by two important features. One is the large spin-dominance \cite{4,5,6}. Nevertheless, silicene distinguish itself from graphene by two important features. One is the large spin-dominance \cite{4,5,6}. The other characteristic is that the lattice structure in silicene is not planar but buckled, with a layer separation between the two sublattices \cite{2}. Thus by introducing a potential difference between the two sublattices one can tune the bandgap \cite{13,14,15,16}. These features imply that in graphene at low energies the electrons behave as massive Dirac fermions \cite{15}, moving with a Fermi velocity of about $5.5 \times 10^5$ m/s \cite{15,16}.

When a magnetic field is applied to silicene, the discrete Landau levels (LL) are obtained. As in graphene, due to the relativistic-like dispersion relation these levels are not equidistant \cite{11}. Moreover, the Landau energy in silicene is smaller than in graphene, due to the bigger Fermi velocity in the latter. The LL create an oscillating behavior in the thermodynamics potentials. For instance, the magnetization oscillates as a function of the inverse magnetic field, the so called de Haas van Alphen (dHvA) effect \cite{20}. The different frequencies involved in the oscillations are related to the closed orbits that electrons perform on the Fermi surface. This effect is purely quantum mechanical and is an useful tool to map the Fermi surface \cite{21}. In graphene it has been found that, without impurities, the magnetization oscillates periodically in a sawtooth pattern \cite{22,23,24}. It is then expected that in silicene the magnetization also oscillates in a sawtooth pattern.

Because of the buckled nature of silicene, by applying a perpendicular electric field the spin and valley degeneracy of the LL is lifted \cite{24}. In this case, in contrast with graphene, the energy levels of each valley are different and there is no more valley degeneracy. Moreover, considering the Zeeman effect, the LL for each spin split, loosing then the spin degeneracy. This loss of valley and spin degeneracy gives discontinuous changes in the last energy level, which in turn is expected to produce new magnetization peaks, as occur in graphene \cite{25}. Motivated by this we have studied the magnetic oscillations (MO) at $T = 0$ K in a general silicene-like system with a conduction electron density $n_e$, which could be due to an applied gate voltage.

We have organized the work as follow: In Sec. 2 we ob-
tain the energy levels of silicene in a perpendicular magnetic and electric field, considering the intrinsic SOI and the Zeeman effect. From this we obtain an expression for the ground state internal energy and magnetization. In Sec. 3 we study and classify the MO peaks for different values of perpendicular electric field. In Sec. 4 we analyze the MO frequencies by performing a fast Fourier transform (FFT). Finally our conclusions follow in Sec. 5.

2. Magnetic oscillations in silicene

2.1. Energy spectrum

In the low wavelength approximation, with energies near the Fermi energy, the electrons in silicene are described by a Dirac-like Hamiltonian in 2D for massive fermions. In a perpendicular electric field $E_z$ it reads \[ H_{qs} = v_F (\sigma_y p_x + \sigma_y p_y) + \sigma_z \Delta_{qs}, \] (1)

where $v_F \sim 5.5 \times 10^5 \text{ m/s}$ is the Fermi velocity, $\sigma_i$ are the Pauli matrices acting in the sublattices $A$ and $B$, $\eta = 1 (-1)$ for the valley $K$ ($K'$), $s = \pm 1$ for spin and down, and

$$ \Delta_{qs} = \eta s \lambda_{SO} - c \ell E_z, $$

where $\lambda_{SO}$ is the intrinsic spin-orbit interaction (SOI) strength and $\ell$ is the buckling height. We shall consider a perpendicular magnetic field $B$, so that $H = B E_z$. In the Landau gauge we have $A = -B y e_z$, and the momentum changes following the Peierls substitution \[ \mathbf{p} \rightarrow \mathbf{p} - e A. \] Considering the Zeeman effect \[ \mu \cdot B = \mu_B B s_z / 2 \]

we get $H_{qs} = \eta s \lambda_{SO} - c \ell E_z$, solving Eq. (1) the energy spectrum results

$$ E_{0,s} = s \lambda_{SO} - e c E_z - s h \omega_Z \quad (n = 0), \quad (7) $$

and

$$ E_{n,\alpha,s} = \beta \sqrt{(s \lambda_{SO} - e c E_z)^2 + (h \omega_L)^2 n} - s h \omega_Z \quad (n \geq 1), \quad (8) $$

where $\beta = -1$ for the valence band (VB) and $\beta = 1$ for the conduction band (CB). When $E_z = 0$, the LL have a doubly valley degeneracy, whereas when $E_z \neq 0$ this degeneracy vanishes. Notice that without the Zeeman effect the LL $n = 0$ is always twice less degenerate than the LL $n \geq 1$, regardless of $E_z$. Therefore the Zeeman effect gives an equal degeneracy for all LL. Moreover, as in the classical case, each LL has a degeneracy due to the free direction ($x$ in this case) which is not quantized. This degeneracy comes by imposing periodical boundary conditions and is given by $D = AB / \varphi$, where $A$ is the silicene sheet area and $\varphi = h / e$ is the magnetic unit flux.

2.2. Ground state magnetization

We shall study the ground state magnetization ($T = 0$ K) for this system, under the influence of a perpendicular magnetic and electric field, where the energy levels are given by Eqs. (7) and (8). We consider a constant electron density $n_e = N / A$, which may due to an applied gate voltage, such that valence band is full and only the conduction band is available. The valence band would still make a continuous (non-oscillatory) contribution to the magnetization, but since we are interested only in the MO, we will not take this contribution into account. The internal energy at $T = 0$ K for the N conduction electrons can be computed as the sum of the filled Landau levels. The number of totally filled levels is $q = \lfloor q_e \rfloor$, where $q_e = N / D$ is the filling factor, and the brackets means the biggest integer less or equal to $q_e$ (Floor function). It is worth noting that we assume that $N$ is constant, instead of the chemical potential $\mu$ (Fermi energy) being constant.

$$ \left[ \frac{\hbar \omega_L}{2} \left( \sigma_+ a_+ \sigma_- a_- \right) + \sigma_z \Delta_{qs} \right] \psi_{qs} = E \psi_{qs}, \quad (5) $$

where $\alpha_1 = a$, $\alpha_2 = a^\dagger$, and $\omega_L = v_F \sqrt{2eB / \hbar}$, $\omega_Z = \mu_B B / 2 \hbar$. The energies can be calculated by writing the wave function for each valley and spin as

$$ | \psi_0^s \rangle = b^s_0 | n, \alpha, s \rangle + c^s_0 | n - \eta, B, s \rangle, \quad (6) $$

where $b^s_0$ and $c^s_0$ are constants, $n$ is the Landau level (LL) index and $| s \rangle = | \pm \rangle$ represents the spin state, so that $s_z | s \rangle = s | s \rangle$. Then, given that $\sigma_+ | A \rangle = 0$, $\sigma_+ | B \rangle = 2 | A \rangle$, $\sigma_- | A \rangle = 2 | B \rangle$, $\sigma_- | B \rangle = 0$, $\sigma_z | A \rangle = | A \rangle$, $\sigma_z | B \rangle = - | B \rangle$ and $a^\dagger | n \rangle = \sqrt{n+1} | n+1 \rangle$, $a | n \rangle = \sqrt{n} | n-1 \rangle$, solving Eq. (5) the energy spectrum results
However, for both cases the results are similar (see the Appendix for details).

In order to compute the ground state internal energy we have to sort the energy levels. We call \( \xi_m \) the decreasing sorted energy levels, \( m = 0, 1, 2 \ldots \) being the label index. In general we write\(^4\)

\[
\xi_m = \sqrt{(s_m \lambda_{SO} - \eta_m \epsilon L)^2 + (\hbar \omega_L)^2 n_m} - s_m \hbar \omega_L,
\]

where \( s_m = \pm 1 \) gives the spin, \( n_m = 0, 1, 2 \ldots \) the LL and \( \eta_m = \pm 1 \) the valley for the \( m \) position. If we denote \( \theta = q_e - q = N/D - [N/D] \) to the occupancy factor of the last unfilled Landau level, the internal energy at \( T = 0 \) K is

\[
U = \sum_{m=0}^{q-1} D \xi_m + D \theta \xi_q.
\]

In Eq. (9) we separate \( \xi_m = \xi^0_m - s_m \hbar \omega_L \), with \( \xi^0_m = \sqrt{(s_m \lambda_{SO} - \eta_m \epsilon L)^2 + (\hbar \omega_L)^2 n_m} \). Replacing in Eq. (10) we can write

\[
U = U_0 - D \hbar \omega_L \left[ \sum_{m=0}^{q-1} s_m + \theta s_q \right],
\]

where

\[
U_0 = \sum_{m=0}^{q-1} D \xi^0_m + D \theta \xi^0_q.
\]

The last term in Eq. (11) can be related to the Pauli paramagnetism associated with the spin population. This can be seen by considering \( N_+ \) and \( N_- \) total number of spin up and down, respectively. For \( q \) levels filled, let \( k_+ \) be the number of \((+1)\) values and \( k_- \) the number of \((-1)\) values in the sorting function \( s_m \), with \( m = 0, 1, \ldots, q - 1 \) (thus \( k_+ \) and \( k_- \) represents the number of spin up and down states totally filled, respectively). Consequently, \( k_+ + k_- = q \) and \( \sum_{m=0}^{q-1} s_m = k_+ - k_- \). For the last unfilled level there could be two cases: (i) it is spin up or (ii) spin down. For spin up, \( s_q = 1 \) and therefore we can write the total number of spin up and down as \( N_+ = D k_+ + D \theta s_q \) and \( N_- = D k_- \). Thus using that \( \sum_{m=0}^{q-1} s_m = k_+ - k_- \) we have \( N_+ - N_- = D \sum_{m=0}^{q-1} s_m + \theta s_q \). The same result holds if the last unfilled level is spin down. Therefore the Pauli magnetization is

\[
M_P = \mu_B (N_+ - N_-) = \mu_B D \left[ \sum_{m=0}^{q-1} s_m + \theta s_q \right].
\]

Notice that this result is independent of how the energy levels are sorted, so that the last term in Eq. (11) is always related to the Pauli paramagnetism. Consequently, because \( \hbar \omega_L = \mu_B B \), Eq. (11) becomes

\[
U = U_0 - BM_P.
\]

The magnetization at \( T = 0 \) K is \( M = -\partial U/\partial B \). From Eq. (11) we have

\[
M = M_0 + M_P + B \partial M_P/\partial B,
\]

where \( M_0 = -\partial U_0/\partial B \). Given that \( \partial D/\partial B = D/B \), \( \partial \theta/\partial B = -N/(DB) \) and \( \partial \xi^0_m/\partial B = (\hbar \omega_L)^2 n_m/2B \xi^0_m = \left[ \sqrt{\xi^0_m} - (s_m \lambda_{SO} - \eta_m \epsilon L)^2/\xi^0_m \right]/2B \), we have

\[
M_0 = \frac{1}{B} \left( N \xi^0_q - \frac{3}{2} U_0 \right) + M',
\]

where

\[
M' = \frac{D}{2B} \left[ \sum_{m=0}^{q-1} (s_m \lambda_{SO} - \eta_m \epsilon L)^2 \xi^0_m \right. + \left. (s_q \lambda_{SO} - \eta_q \epsilon L)^2 \xi^0_q \right]/\xi^0_q.
\]

This new contribution \( M' \) to the magnetization is not present in graphene\(^2\) due to the negligible SOI and zero buckle height. On the other hand, from Eq. (11) we get \( \partial M_P/\partial B = M_P/B + \mu_B D s_q \partial \eta_q/\partial B = (M_P - \mu_B N s_q)/B \). Therefore, from Eqs. (9), (14) and (15), the total ground state magnetization given by Eq. (11) can be written as

\[
M = \frac{1}{B} \left( N \xi_q - \frac{3}{2} U_0 \right) + M' + \frac{1}{2} M_P.
\]

This is the fundamental equation for our analysis. It shows that the MO peaks are produced whenever \( \xi_q, M' \) or \( M_P \) changes discontinuously, \( U \) being continuous always. Thus the magnetization in pristine silicene at \( T = 0 \) K oscillates in a sawtooth pattern, as in graphene\(^2\)^\(^2\) and in general 2DEG with a Dirac-like spectrum\(^2\). This is also in agreement with the results found in\(^2\), where the MO at \( T = 0 \) K in a pristine buckled honeycomb lattice are expressed as an infinite sum of harmonics \( k \) of the form \( \sin(k)/k \), which gives a sawtooth oscillation. From Eq. (13) we write the MO peak amplitude \( \Delta M \) as

\[
\Delta M = \frac{N}{B} \Delta \xi_q + \Delta M' + \frac{1}{2} \Delta M_P.
\]

The first contribution \( \Delta \xi_q \) comes directly from the discontinuous change in the last energy level, which occurs only when the filling factor \( q \) changes. On the other hand, by analyzing Eqs. (13) and (17) we see that the MO peaks produced by \( \Delta M' \) and/or \( \Delta M_P \) occur when the parameters \( \eta_q \) and \( s_q \) change but \( \xi_q \) remains continuous. This

\(^{1}\)For the LL \( n = 0 \) only the positive root should be taken. See Eq. (4).
would happen if the change in \( q \) and \( s_q \) does not come from a change in the filling factor \( q \).

Eq. 18 also allows an intuitive interpretation of the effect that impurities have in the magnetization. In the pristine case, the discontinuities in \( \xi_q \), \( M' \) or \( M_P \) are essentially a product of the discrete LL, which gives a delta-like density of states (DOS) and causes the MO to be sawtooth-like. But when impurities are added to the system, the DOS is broadened and the discontinuities in \( \xi_q \), \( M' \) or \( M_P \) disappear. Consequently, the MO are also broaden and the oscillations are no more sawtooth-like.

2.3. LL, valley and spin mixing

We are interested in how the parameters \( n_q \), \( \eta_q \) and \( s_q \) vary with \( B \) for different values of \( e\ell E_z \). We recall that \( n_q \) may take values 0, 1, 2, \ldots, while \( \eta_m = 1 (-1) \) for the \( K (K') \) valley and \( s_m = 1 (-1) \) for spin up (down). The value of these parameters depends on the sorted position \( q \), which in turn depends in the mixing of the LL, valley and spin. We consider a conduction electron density \( n_e = 0.01 \text{ nm}^{-2} \) and an area \( A = 1000 \text{ nm}^2 \). In Fig. 1 we show the parameters \( n_q \), \( \eta_q \) and \( s_q \) as a function of \( B \) for different values of \( e\ell E_z \).

In Fig. 1(a) we can see the case \( E_z = 0 \), where there is no parameter \( \eta_q \) because each energy level in Eq. 19 has a doubly valley degeneracy. The last energy level \( \xi_q \) changes discontinuously only whenever the LL \( n_q \), the spin \( s_q \) or both change. When \( E_z \neq 0 \), the valley degeneracy is broken and the energy levels start to depend on \( \eta_q \). This can be seen in Fig. 1(b), where for \( e\ell E_z = 5 \text{ meV} \) the parameters start to vary differently. Nevertheless, it should be noted that in both Fig. 1(a) and 1(b) there is no appreciable mixing of the parameters. This means that in each case \( n_q \) is always decreasing (as \( B \) is increased), while \( \eta_q \) and \( s_q \) alternate in the same way between -1 and 1. Moreover, in either case both \( M' \) and \( M_P \) are always continuous because every change in the parameters is produced by a change in the filling factor \( q \), so \( \Delta M' = 0 = \Delta M_P \) in Eq. 19. As \( E_z \) increases, the parameters start to vary in a more complicated way. This can be seen in Fig. 1(c), in the case \( e\ell E_z = 64 \text{ meV} \), where there is a notorious mixing of the parameters, which implies that \( M' \) and \( M_P \) may not be always continuous. In such case all three contributions in Eq. 19 will be present.

3. Classification of MO peaks

We showed in Eq. 18 that the MO peaks are produced by the discontinuous changes in \( \xi_q \), \( M' \) or \( M_P \), which in turn depends on \( n_q \), \( \eta_q \) and \( s_q \). This allows a classification of the MO peaks according to the parameters that change. We can define seven general types of peaks, considering the change of LL, valley or spin and its combinations. This can be seen in Table 1.

Furthermore, each type of MO peak has its own subpeaks, corresponding to different possible ways in which the parameters can change. The type of subpeak can be identified from the change in \( n_q \), \( \eta_q \) and \( s_q \). In general we label the subpeaks as \( X^{\pi}_{\pi'} \), where \( X = \{ L, LV, LS, LVS, V, VS, S \} \) identifies the type of MO peaks, as classify in Table 1, and \( \pi, \pi' \) and \( \pi' \) indicate the change (or not) of the parameters. For example, consider an LS peak corresponding to a change of LL \( n = 5 \rightarrow 4 \) and spin \( \uparrow \uparrow \rightarrow \uparrow \downarrow \) in the valley \( K \). Then we identify this peak with \( \text{LS}_{K,\uparrow \uparrow \rightarrow \uparrow \downarrow} \).

The defined classification of MO peaks provides a systematic way of recognizing them in a magnetization graph. One procedure could be to first analyze how the energy levels are sorted (as done in Sec. II.C), from which one could predict which type of MO peak appear and in which order. We shall do this first for the case \( e\ell E_z \ll 1 \text{ eV} \), and then for the general case in which \( e\ell E_z \) may take any value. In
all cases we shall take $0.6 < B[T] < 0.685$, as in Fig. 1.

3.1. Limit $e\ell E_z \ll 1$ eV

We consider low $e\ell E_z$ such that the parameters change only when the filling factor $q$ does it. Hence in this regime both $M'$ and $M_{\rho}$ are continuous and only $\Delta \xi_{q\ell}$ contributes to the MO peaks in Eq. (19). We will consider the cases $E_z = 0$ and $e\ell E_z = 5$ meV, when the sorting of the parameters is given by Fig. 1. Then, following the classification of Table 1, we see in Fig. 1(a) that the possible type of MO peaks at $E_z = 0$ are LS and S, with the order LS, S, L, S,... On the other hand, we see in Fig. 1(b) that at $e\ell E_z = 5$ meV the MO peaks are LS, VS and S, with the order LS, VS, S, VS, L,... These results can be seen in Fig. 2 where we plot the magnetization (18) for $E_z = 0$ and $e\ell E_z = 5$ meV.

For $E_z = 0$ we effectively see that only the peaks LS and S appear. The S peaks always correspond to a change of spin down to up, so its amplitude is always $\Delta M = 2N_\mu_B$ at $E_z = 0$. When $e\ell E_z = 5$ meV, the VS peak appears, and the order of the peaks is LS, VS, S, VS, S,..., as expected. The LS peak always correspond to a change of spin up to down in a K valley. The VS peak corresponds to $\{K \rightarrow K', \downarrow \rightarrow \uparrow\}$ or $\{K' \rightarrow K, \downarrow \rightarrow \uparrow\}$, while the S peak always correspond to a change of spin up to down in the $K'$ valley. Thus, from Eqs. (9) and (10) we can write the corresponding peaks amplitude

$$\Delta M_{LS} = \frac{N}{B} \left[ \chi(n_q; -e\ell E_z) - \chi(n_q - 1; +e\ell E_z) \right] - 2N_\mu_B, \quad (20)$$

$$\Delta M_{VS} = \frac{2N_\mu_B}{B}, \quad (21)$$

$$\Delta M_S = \frac{N}{B} \left[ \chi(n_q; +e\ell E_z) - \chi(n_q - 1; -e\ell E_z) \right] - 2N_\mu_B, \quad (22)$$

where $\chi(n_q; \pm e\ell E_z) = \sqrt{(\lambda_{SO} \pm e\ell E_z)^2 + (\hbar \omega_L)^2} n_q$, with $n_q$ being the corresponding LL level, as indicated in Fig. 2. The VS peak always has the same amplitude $2N_\mu_B$, which is equal to $\Delta M_{\rho}$ in the case $E_z = 0$. In the limit $e\ell E_z \ll 1$ we can approximate the subpeaks amplitude in Eqs. (20) and (22) by

$$\frac{B}{N} \Delta M_{LS} \approx \varrho_+ - 2\hbar \omega_z - \lambda_{SO} e\ell E_z \varrho_-,$$  

$$\frac{B}{N} \Delta M_S \approx [\gamma_q^{-1}(\lambda_{SO}, \omega_L) 2\lambda_{SO}] e\ell E_z - 2\hbar \omega_z,$$  

where $\varrho_{\pm} = \gamma_{q\pm}^{\pm}(\lambda_{SO}, \omega_L) \pm \gamma_{q\pm}^{-1}(\lambda_{SO}, \omega_L)$, with $\gamma_q(\lambda_{SO}, \omega_L) \equiv \sqrt{\lambda_{SO}^2 + (\hbar \omega_L)^2} n_q$. Thus the peak amplitudes is linear with $E_z$, with both the slope and the y-intercept depending on $\lambda_{SO}$ and $\omega_L$. By studying how the amplitude of the peaks vary with $E_z$, one could obtain the parameters $\lambda_{SO}$ and $\omega_L$, provided that the magnetic field $B$ and $n_q$ of the peaks are known. It is important to notice that for each peak the magnetic field $B$ and $n_q$ are different. The Landau level $n_q$ could be inferred knowing

| LL change | Valley change | Spin change | Type of MO peak |
|-----------|---------------|-------------|----------------|
| ✓         | ×             | ×           | L             |
| ✓         | ✓             | ×           | LS            |
| ✓         | ×             | ✓           | Vs            |
| ×         | ✓             | ×           | V             |
| ×         | ×             | ✓           | S             |
| ×         | ×             | ✓           | S             |

Table 1: Classification of MO peaks according to the change in the parameters $n_q$ (LL), $n_q$ (valley) and $s_q$ (spin).

Figure 2: Magnetization given by Eq. (18) for (a) $E_z = 0$ and (b) $e\ell E_z = 5$ meV.
at which $B$ the type of peak occur, and how is the sorting of the energy levels. For instance, when $eE_z = 5$ meV, we know that the sorting is given by Fig. 1(b). Thus, the second peak LS in Fig. 2(b) corresponds to a change of LL from $n = 16 \rightarrow 15$, so we put $n_q = 16$ in Eq. (23).

This way of obtaining $\lambda_{SO}$ and $\omega_L$ from the MO peaks could be an useful alternative to the other available methods. The Landau energy $\omega_L$ gives the Fermi velocity, since we define $\omega_L = v_F \sqrt{2eB/\hbar}$. In silicene, the Fermi velocity has usually been obtained using DFT or TB models, with the result of a lower value than in graphene [4, 6, 18]. This can be easily understood from the reduced hopping in silicene since the Si atoms are more distant from each other.

Likewise, the SO parameter $\lambda_{SO}$ is usually obtained from TB models using the hopping parameters [7].

3.2. General case

In the general case the mixing of the parameters $n_q$, $\eta_q$ and $s_q$ depends on the specific value of $eE_z$. We saw in Fig. 1(c) that these parameters vary in a complicated way as $eE_z$ increases. Thus for any specific value of electric field one should see how the energy levels are sorted in order to identify the MO peaks. Moreover, in the general case $M'$ and $M_P$ may no longer be continuous, and the contributions $\Delta M'$ and $\Delta M_P$ should be taken into account in Eq. (19).

We consider $eE_z = 64$ meV, in which case $n_q$, $\eta_q$ and $s_q$ as a function of $B$ are given in Fig. 1(c). Then we can identify ten MO peaks for $0.6 < B(T) < 0.685$. For instance, the first is a LS peak corresponding to $\{K, \uparrow \rightarrow \downarrow\}$, while the sixth is a VS peak corresponding to $\{K \rightarrow K', \downarrow \rightarrow \uparrow\}$. In the same way one can classify the other peaks, leading to the magnetization for $eE_z = 64$ meV shown in Fig. 3.

As we see, the mixing of the parameters alters drastically the magnetization. In particular we note that in the two peaks $LV_{18 \rightarrow 14}^{K \rightarrow K', \downarrow \rightarrow \uparrow}$ and $LS_{18 \rightarrow 14}^{K \rightarrow K', \downarrow \rightarrow \uparrow}$ the magnetization increases, which is opposite to all other peaks, where the magnetization always decreases. This feature suggests that the peaks $LV_{18 \rightarrow 14}^{K \rightarrow K', \downarrow \rightarrow \uparrow}$ and $LS_{18 \rightarrow 14}^{K \rightarrow K', \downarrow \rightarrow \uparrow}$ are not produced by the change $\Delta \zeta_q$, but come from the discontinuities in $M'$ and $M_P$. Indeed, the contribution $\Delta \zeta_q$ always lower the magnetization because it comes from the discontinuous change in the last energy level $\zeta_q$ as $B$ increases. To see this we plot in Fig. 4 the variation of $\zeta_q$, $M'$ and $M_P$ with respect to $B$, for $eE_z = 64$ meV.

We can clearly appreciate two discontinuities in $M'$ and one discontinuity in $M_P$. We also see that when these discontinuities occur $\zeta_q$ is continuous, which implies $\Delta \zeta_q = 0$. Thus the peaks $LV_{18 \rightarrow 14}^{K \rightarrow K', \downarrow \rightarrow \uparrow}$ and $LS_{18 \rightarrow 14}^{K \rightarrow K', \downarrow \rightarrow \uparrow}$ are

\[\text{Nevertheless we can see that the slope of } \zeta_q \text{ slightly changes}\]
effectively produced by $\Delta M'$ and $\Delta M_p$. The first peak LV$^{18\rightarrow14}_{K'\rightarrow K}$ only has contribution from $\Delta M'$ because only the valley changes. This can be seen in Fig. 4, where when the first discontinuity occurs in $M'$ we see that $M_p$ is continuous. On the other hand, the peak LS$^{18\rightarrow14}_{K'\uparrow\rightarrow K\downarrow}$ has both contributions $\Delta M'$ and $\Delta M_p$, as can be seen in Fig. 4, where both $M'$ and $M_p$ have a discontinuity. In this way we can say, in general, that the MO peaks that increase the magnetization are not produced by the discontinuous change in the last energy level $\xi_q$, but rather by the discontinuous change in $M'$ and/or $M_p$.

4. MO frequencies

So far we have analyzed only the MO peaks amplitude, but we can also obtain information from their frequencies. For simplicity we shall consider the cases $E_z = 0$ and $e\ell E_z = 5\text{ meV}$, such that the only contribution in Eq. (19) is given by $\Delta \xi_q$ and all the MO peaks can occur only when the filling factor $q$ changes. Given that $q = [N/D] = [n_e\varphi/B]$, it is clear that the magnetization oscillates periodically as a function of $1/B$, in agreement with the Onsager relation [21]. The period of oscillation is in general given by $\Delta (1/B) = 1/B_2 - 1/B_1$, where $B_1 = n_e\varphi/q_1$ and $B_2 = n_e\varphi/q_2$ ($\varphi = h/e$). Thus we can write

$$\Delta \left( \frac{1}{B} \right) = \frac{e}{2\pi\hbar n_e} \Delta q,$$  \hspace{1cm} (25)

where $\Delta q = q_2 - q_1$. Because the MO are sawtooth like, there will be many frequencies involved in its Fourier expansion. Nevertheless we are interested only in the fundamental frequencies, for the others are just harmonics of these ones. To obtain the frequency spectrum we performed a fast Fourier transform (FFT) in the magnetization as a function of $1/B$.

In Fig. 5 we can appreciate the case $E_z = 0$, where the MO are a combination of two sawtooth oscillations (SO) with different frequencies, as can be inferred in the FFT spectrum, where two main frequencies $\omega_1 = 10.33\text{ T}$ and $\omega_2 = 20.67\text{ T}$ can be recognized. This can be explained if we decompose the term $\xi_q$ in Eq. (19), which causes the SO with its discontinuous change. When $E_z = 0$ we have, from Eq. (10), $\xi_q = \sqrt{\xi_{SO}^2 + (n\omega Z)^2 n_q - s_q\hbar\omega Z} = \xi^L_q - \xi^S_q$, where we separated

when $M'$ or $M_p$ are discontinuous. The reason for this is that the variation of the parameters in this places do modify $\xi_q$, but in a continuous way, giving a different dependence with $B$ without any discontinuous jump.

Figure 5: Magnetization and fast Fourier transform (FFT) for $E_z = 0$.

Figure 6: Magnetization and fast Fourier transform (FFT) for $e\ell E_z = 5\text{ meV}$. 

$\xi_{SO}$
\[ \xi^L_q = \sqrt{\lambda^2_{SO} + (\hbar \omega L)^2} n_q, \quad (26) \]
\[ \xi^S_q = s_q \hbar \omega_z. \quad (27) \]

The term \( \xi^L_q \) is only related to the LL, while the term \( \xi^S_q \) is only related to the spin. Then, considering the parameters sorting given by Fig. 1(a), and taking into account the valley degeneracy at \( E_z = 0 \), we get that \( \xi^L_q \) changes periodically when \( q \) changes by four, so \( \Delta q = 4 \) in Eq. (25), giving the frequency \( \omega_1 = \pi \hbar n_e / 2e \). On the other hand, \( \xi^S_q \) changes periodically when \( q \) changes by two, so \( \Delta q = 2 \) in Eq. (25), giving the frequency \( \omega_2 = \pi \hbar n_e / e \). Thus the magnetization in Eq. (15) can be decomposed in two SO with two different fundamental frequencies. For the considered electron density \( n_e = 0.01 \text{ nm}^{-2} \) we obtain \( \omega_1 = 10.34 \text{ T} \) and \( \omega_2 = 20.68 \text{ T} \), in agreement with Fig. 5.

When \( \epsilon E_z = 5 \) meV the valley degeneracy is broken, which gives rise to another MO frequency \( \omega_3 = 41.33 \text{ T} \), as seen in Fig. 6. The origin of this can be explained by first approximating \( \xi^L_q \) for low \( \epsilon E_z \), so \( \xi^L_q \approx \sqrt{\lambda^2_{SO} + (\hbar \omega L)^2} n_q - s_q \hbar \omega_z - \epsilon E_z \lambda_{SO} \eta_q \eta_q \left[ \lambda^2_{SO} + (\hbar \omega L)^2 n_q \right]^{-1/2} \). This can be separated as \( \xi^L_q = \xi^L_q - \xi^S_q - \xi^V_S \), where \( \xi^L_q \) and \( \xi^S_q \) are given by Eqs. (26) and (27), while

\[ \xi^V_S = \epsilon E_z \frac{\lambda_{SO} \eta_q n_q}{\sqrt{\lambda^2_{SO} + (\hbar \omega L)^2 n_q}} \quad (28) \]

For \( \epsilon E_z = 5 \) meV, the sorting of the parameters \( n_q \), \( \eta_q \) and \( s_q \) is given by Fig. 1(b). Hence \( n_q \) still changes only \( q \) changes by four, so \( \xi^L_q \) gives the frequency \( \omega_1 = \pi \hbar n_e / 2e \approx 10.34 \text{ T} \). On the other hand, now \( s_q \) changes whenever \( q \) changes, so for \( \xi^S_q \) we have \( \Delta q = 2 \) in Eq. (25). This gives a new frequency \( \omega_3 = 2 \pi \hbar n_e / e \) which implies \( \omega_3 = 41.36 \text{ T} \) for \( n_e = 0.01 \text{ nm}^{-2} \). Finally, the new defined term \( \xi^V_S \) in Eq. (28) changes discontinuously when \( \Delta q = 2 \), as can be easily seen in Fig. 1(b). Therefore we also have the frequency \( \omega_2 = \pi \hbar n_e / e = 20.68 \text{ T} \).

5. Conclusions

We studied the magnetic oscillations (MO) in pristine silicon at \( T = 0 \text{ K} \). We considered a constant electron density, such that the valence band is full and only the conduction band is available. Under a perpendicular electric and magnetic field, we found analytical expressions for the ground state internal energy and magnetization. We obtained that the MO are sawtooth-like and are entirely produced by the change in the last energy level occupied. This lead us to a classification of the MO peaks in terms of the parameters \( n_q \) (LL), \( \eta_q \) (valley) and \( s_q \) (spin) which define the last energy level. In general we defined seven types of MO peaks, as indicated in Table 1. Using this classification we analyzed the MO in the case of low electric field \( (\epsilon E_z \ll 1 \text{ eV}) \), and the general case in which \( E_z \) may take any value. In each case we were able to classify the type of MO present, and in which order. When \( E_z = 0 \) the energy levels have a valley degeneracy and the MO peaks occur only when the last occupied level changes its LL and/or spin. On the other hand, when \( E_z \neq 0 \) the valley degeneracy is broken and new MO peaks appear, associated with the change of the valley in the last energy level. Furthermore, we found that analyzing the MO peak amplitude one could extract information about the Fermi velocity and the spin-orbit interaction strength, which could be an useful alternative to the other available methods.

For the general case of \( E_z \) the last energy level varies in a complicated way and therefore so does it the MO peaks. Nevertheless one can still classify the peaks by studying the change in the parameters \( n_q \), \( \eta_q \) and \( s_q \) at any particular \( E_z \). Finally we analyzed the MO frequencies, where we found that the magnetization effectively oscillates periodically a function of \( 1 / B \). We performed the fast Fourier transform spectrum of the sawtooth-like MO oscillations. When \( E_z = 0 \) we found two fundamental frequencies, corresponding to the change of LL or spin in the last energy level. When \( \epsilon E_z = 5 \) meV a new fundamental frequency appears, associated with broken valley degeneracy.

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Appendix A. Magnetization for constant Fermi energy

We shall analyze the case in which the Fermi energy \( \mu \) is held constant, instead of the conduction electron density \( n_e \). We consider \( \mu > 0 \) such that last energy level filled always correspond to the CB. The valence band is not taken into account since it is full and thus will not contribute to the MO. Because we consider \( \mu \) fixed, whereas the number of electrons \( N \) may change, we work with the grand potential \( \Omega \). For a Fermi energy \( \mu \), all energies levels \( m = 0, 1, 2 \ldots m_F \) all filled, where \( m_F \) is such that \( \xi_{m_F} \leq \mu \leq \xi_{m_{F+1}} \). Then the grand potential \( \Omega \) at \( T = 0 \text{ K} \) is

\[ \Omega = \sum_{m=0}^{m_F} D (\xi_m - \mu), \quad (A.1) \]
where $\xi_m$ is given by Eq. (9). Separating $\xi_m = \xi_m^0 - s_m \hbar \omega_z$, with $\xi_m^0 = \sqrt{(s_m \lambda_{SO} - \eta_m e \epsilon E_z)^2 + (\hbar \omega_l)^2} n_m$, we get

$$\Omega = \Omega_0 - D \hbar \omega_z \sum_{m=0}^{\infty} s_m,$$

(A.2)

where

$$\Omega_0 = \sum_{m=0}^{m_F} D (\xi_m^0 - \mu).$$

(A.3)

As in the case with $N$ constant, the last term in Eq. (A.2) is related to the Pauli paramagnetism associated with the spin population, with the difference that this time all the energy levels below the Fermi energy are completely filled. Thus the Pauli paramagnetism is $M_P = \mu_B (N_+ - N_-) = \mu_B D \sum_{m=0}^{m_F} s_m$, and Eq. (A.3) becomes

$$\Omega = \Omega_0 - BM_P.$$

(A.4)

This result is similar to the one obtained in Eq. (14), with $U$ being replaced by $\Omega$. Therefore, similar expressions are obtained for the magnetization, given by $M = - (\partial \Omega/\partial B)_\mu$. From Eq. (A.4) we obtain

$$M = -\frac{1}{2B} (3\Omega + N\mu + M' + \frac{1}{2} M_P),$$

(A.5)

where $N = \sum_{m=0}^{m_F} D = D (m_F + 1)$ is the number of electrons, and

$$M' = \frac{D}{2B} \sum_{m=0}^{m_F} \frac{(s_m \lambda_{SO} - \eta_m e \epsilon E_z)^2}{\xi_m^0}.$$

(A.6)

Eq. (A.5) shows that, when $\mu$ is constant, the MO peaks are produced whenever $N$, $M'$ or $M_P$ changes discontinuously, with $\Omega$ being continuous always. Then in general we write the MO peak amplitude $\Delta M$ as

$$\Delta M = -\frac{\mu}{2B} \Delta N + \Delta M' + \frac{1}{2} \Delta M_P.$$

(A.7)

This last equation is similar to Eq. (19), with each contribution $\Delta N$, $\Delta M'$ and $\Delta M_P$ being still defined by the discontinuous change in the parameters $n_q$, $n_y$ and $s_q$. The main difference is that in this case, with $\mu$ constant, all the three functions $N$, $M'$ and $M_P$ have discontinuities at any $E_z$. Nevertheless, one could still classify the MO peaks as done in Table 1, which accounts for the main results found in the case when $N$ is constant.

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