Abstract We consider quasi-two-dimensional gas of electrons in a typical Si-MOSFET, assuming repulsive contact interaction between electrons. Magnetisation and susceptibility are evaluated within the mean-field approach. Finite thickness of the inversion layer results in an interaction-induced electron wave function change, not found in both purely two-dimensional and three-dimensional (bulk) cases. Taking this self-consistent change into account leads to an increased susceptibility and ultimately to a ferromagnetic transition deep in the high-density metallic regime. We further find that in the paramagnetic state, magnetisation increases sublinearly with increasing in-plane magnetic field. In the opposite limit of low carrier densities, the effects of long-range interaction become important and can be included phenomenologically via bandwidth renormalisation. Our treatment then suggests that with decreasing density, the metal-insulator transition is preceded by a ferromagnetic instability. Results are discussed in the context of the available experimental data, and arguments for the validity of our mean-field scheme are presented.

Keywords MOSFET · 2DEG · magnetic properties · ferromagnetism

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1 Introduction

Silicon metal-oxide-semiconductor field-effect transistors (Si-MOSFETs) have been in the focus of an extensive research effort throughout the ongoing studies of the properties of low-dimensional electron systems. Fifty years ago, electrons in the Si-MOSFET inversion layers\[1\] were among the first experimental realisations of 2-dimensional (2D) electron gas (2DEG)\[2\]. Some thirty years
later, they yielded the first example of a metal-insulator transition (MIT) in a 2D system [3,4]. While the full understanding of this phenomenon is yet to be achieved, a remarkable progress toward this goal has been made both experimentally and theoretically [5]. In particular, attention was paid to the close interplay between spin and charge degrees of freedom, as exemplified by strong positive magnetoresistance in a parallel magnetic field (when orbital effects are negligible) [4,6]. This allows, for example, to use an electric current for manipulating the spin density in restricted geometries [7], which appears relevant in the general context of spintronics.

As opposed to the magnetotransport, measuring the magnetic properties of the 2DEG presents formidable experimental difficulties [8,9,10]. In the case of Si-MOSFETs, such measurements are necessarily indirect, and both accuracy and interpretation of the results can and should be questioned. Nevertheless, it was established that the low-field magnetic susceptibility in the metallic state increases when the carrier density (controlled by a voltage applied to the metallic gate) is decreased toward the MIT. It is not yet reliably verified whether this increase is finite [11], or a ferromagnetic transition takes place in the vicinity of the MIT [5,9]; in addition, evidence of magnetic inhomogeneities has been reported recently for low densities [12]. An important theoretical study suggests a divergence of the electron effective mass and hence of the susceptibility at the MIT without an associated magnetic transition [13].

It should be noted that the possibility of ferromagnetism in a 2DEG is a fascinating subject in itself, originally suggested on the basis of numerical investigations [14]. While this suggestion finds further support in some subsequent numerical work [15], others [16] do not find any critical behaviour of susceptibility in a low density two-valley 2DEG (the latter, as appropriate for a Si-{100} MOSFET). It was also noted that in reality, the inversion layer has a finite thickness (which increases for smaller carrier densities), resulting in a quasi-2DEG (as opposed to a strictly 2D case). This was taken into account by including the appropriate formfactors [2] into diagrammatic summations [17,18] and Monte-Carlo numerical calculations [19,20]. Orbital effects of the in-plane magnetic field were invoked as well [21].

Thus, the magnetic properties of 2DEG in Si-MOSFETs attract considerable attention from both theorists and experimentalists. It is therefore somewhat surprising that a systematic Stoner-type mean field treatment has not been carried out for this case. This is probably due to the fact that in a 2DEG at low densities (in the vicinity of the MIT), the dominant role is played by the long-range Coulomb correlations, whereas the Stoner approach emphasises the local mean field, arising from the short-range (or on-site) repulsion.

In agreement with Ref. [13], a comprehensive recent review [22] of experimental data finds a pronounced renormalisation of quasiparticle band on approaching the MIT from the high-density metallic phase. Phenomenologically, the data correspond to a non-interacting 2DEG with a bandwidth vanishing at the MIT. We argue that the effects of the short-range interaction likely become important in this case, drastically modifying the magnetic properties of the system and leading to a ferromagnetic transition. This surely holds also
in the opposite case of high carrier density (deep inside the metallic phase): there, the on-site repulsion provides the dominant contribution to magnetic susceptibility, which increases with density. Due to the restricted geometry of electron motion in MOSFETs (finite layer thickness), the mean field theory takes on a somewhat unusual form as opposed to purely 2D or 3D cases. In addition to Zeeman-like energy shifts under a combined effect of interaction and external field, one must take into account changes in the carrier wave functions. This effect, which was not included in previous treatments, leads to a further increase in susceptibility. This opens an intriguing possibility of a ferromagnetic transition in the region where the interaction is still not too strong, and hence the mean field approach is qualitatively valid. The latter should be contrasted with the well-known failure of mean field theory for the two-dimensional Hubbard model, where even in the case of infinite on-site repulsion ferromagnetism may arise only in a restricted range of values of the carrier density\[23,24,25\] (although the ferromagnetic region of the phase diagram is broadened once the allowance is made for further-neighbour hopping\[26\] and for partial spin-polarisation in the ferromagnetic state\[27\]). On the other hand, we note recent results\[28\] on 2D atomic gases with short-range repulsion, suggesting that mean field theory may be overestimating the interaction strength required for ferromagnetism.

For the purposes of the present study, it is obviously important to adequately estimate the strength of short-range interaction. While a recent article\[29\] suggests that the on-site repulsion is of order $U_{on-site} \approx 3$ eV, this is likely to be an over-estimate, especially since the Wannier function in silicon can be expected to spread over several lattice sites. On the other hand, we wish to write the short-range interaction $U_{3D}$ for our continuum description in the form of a contact repulsion (or equivalently an $s$-wave scattering),

$$U_{3D} = U \delta(x - x') \delta(y - y') \delta(z - z').$$

(1)

Interaction constant $U$ includes contributions from those neighbouring sites $j$ on the underlying discrete lattice where the wavefunction overlap with a given site $i$ (or equivalently, the off-site repulsion $U_{ij}$) is non-negligible\[3\]:

$$U \sim a^3 \sum_j U_{ij}, \quad U_{ii} \equiv U_{on-site},$$

(2)

with $a \approx 5.43$ Å the lattice period. Taking the simple cubic lattice as an example, we see that the combined effect of a rather more realistic $U_{on-site} \sim 0.75$ eV, the nearest neighbour $U_{ij} \sim 0.25$ eV and next-nearest neighbour repulsion of $U_{ij} \sim 0.1$ eV is the same as that of a $U_{on-site} = 3$ eV acting alone. Given the apparent absence of reliable ab initio data for $U_{ij}$, we will be using the latter estimate henceforth.

1 While any $U_{ij} \neq 0$ with $i \neq j$ would also lead to an interaction between same-spin carriers, it obviously cannot give rise to an $s$-wave repulsion between these. The effects of $p$-wave and higher harmonics can be expected to be weak and will be neglected.
The outline of the present paper is as follows. The model and the mean field scheme are introduced in Sect. 2. In the following section, we analyse the mean field solution in the low- to moderate density range, where only one transverse level is occupied, discussing the emergent behaviour and also comparing it to a simple variational result. As explained above, when approaching the MIT one has to take into account the bandwidth renormalisation due to the long-range interactions (Sect. 4). In the opposite regime of large densities, a proper description implies filling multiple transverse levels, as described in Sect. 5. We note that our results suggest a possibility of ferromagnetism in both cases. The field dependence of magnetisation in the paramagnetic phase is discussed in Sect. 6 and the concluding discussion is relegated to Sect. 7. Our analysis relies on a conjecture that the Stoner approach remains relevant in a 2D system down to sufficiently low densities. Arguments to this effect are given in the Appendix.

Early preliminary results were reported in Ref. [30].

2 Si-MOSFET inversion layer, and the mean field scheme

Here, we generalise the familiar mean-field description[31] of an n-doped Si inversion layer, taking into account the short-range electron-electron repulsion and allowing for the presence of an applied magnetic field.

In a Si-MOSFET, a quasi-2D conducting layer is formed on the surface of bulk silicon, and the spectral properties of the carriers depend on the crystallographic orientation of this surface. While this is not expected to affect our results at the qualitative level, we consider the case of a \{100\} surface. When a sufficiently large positive voltage $\phi_{gate}$ is applied to the metallic gate (which is separated from Si by an oxide layer, see schematics in Fig. 1), conduction band valleys dip below the Fermi level. The latter is fixed at the top of the valence band of the bulk Si, which we will use as a zero of energy, $E_v = 0$. An adequate description of electrostatics cannot be achieved without taking into account the impurities present in the bulk. Again, it is expected that the details are unimportant and we assume the presence of a single acceptor
level at $E = 0$ (more precisely, at a negligible positive $E$), with the volume density of acceptors $N_A$. When a small positive voltage $\phi_{\text{gate}}$ is applied to the gate, a depletion layer of variable width $z_d$ is formed near the surface. Within this layer (at $z < z_d$, assuming $z = 0$ at the surface), the acceptor states are occupied by electrons, whereas the bottom of the conduction band decreases linearly from its bulk value $E_c$ to a (variable) value $E_{cs}$ achieved at $z = 0$ (triangular potential; note that we consider the case of zero temperature). Equivalently, the electrostatic potential $\phi(z)$ increases linearly from its constant value (which we choose as $\phi = 0$) within the bulk (i.e., everywhere at $z > z_d$). With increasing $\phi_{\text{gate}}$, the value of $E_{cs}$ becomes negative; at a certain point thereafter, the lowest electronic states in the quantum-mechanical potential well formed by the bent conduction-band bottom (see below) drop below $E = 0$ and the quasi-2D electron gas (Q2DEG) with two-dimensional carrier density $n$ is formed. Throughout, the value of $E_{cs}$ is self-consistently determined by a condition

$$\phi(z = 0) \equiv -\frac{1}{e}(E_{cs} - E_c) = -\frac{1}{C}Q_{\text{gate}} + \phi_{\text{gate}},$$

(3)

where $-e$ is the electron charge, and $Q_{\text{gate}}$ is the (positive) surface charge density at the gate, which is exactly compensated by the induced charges in the semiconductor: $Q_{\text{gate}} = e(n + N_A z_d)$. $C$ is the capacitance per unit area of the oxide layer,

$$C = 4\pi \varepsilon_{\text{ox}} / d_{\text{ox}}$$

where $\varepsilon_{\text{ox}}$ and $d_{\text{ox}}$ are the dielectric constant of SiO$_2$ and the layer thickness.

We will be interested in the case where $n$ exceeds the critical value $n_0$ corresponding to the MIT. In this regime, $n$ is of the same order or larger than the two-dimensional density of depletion layer charge $N_A z_d$, and the potential felt by the mobile carriers can no longer be approximated by a triangular one; instead, we must solve a self-consistent Poisson equation, which for $0 < z < z_d$ takes form:

$$\frac{d^2\phi(z)}{dz^2} = 4\pi e \left[ N_A + \sum_{l,a,\alpha} n_{l,a,\alpha} \psi_{l,a,\alpha}^2(z) \right],$$

(4)

where $\varepsilon$ is the static dielectric constant of Si. The charge density on the r.h.s. includes contributions from acceptors and from the Q2DEG carriers; the latter are subdivided according to the number of the corresponding transverse-motion level $a = 0, 1, 2, \ldots$ within the “ladder” $l$ (with $l = 0, 1$, see below), and the spin index $\alpha = \uparrow, \downarrow$. The corresponding 2D carrier densities and wave functions of transverse motion are denoted $n_{l,a,\alpha}$ and $\psi_{l,a,\alpha}$ (with $\int_0^\infty \psi_{l,a,\alpha}^2(z) dz = 1$). The net densities of spin-up and -down electrons will be denoted by $n_{\alpha}$, so that

$$n_{\alpha} = \sum_{l,a} n_{l,a,\alpha}, \quad n = n_{\uparrow} + n_{\downarrow}, \quad M = \frac{n_{\uparrow} - n_{\downarrow}}{2},$$

(5)
where \( M \) is magnetisation density in units of the Bohr magnetone. We will be interested in the effects of in-plane magnetic field, in which case the spin-quantisation axis lies parallel to the Q2DEG plane (\( xy \)-plane).

The value of electric field at the surface is found from the Gauss theorem as
\[
\mathcal{E}(z = 0) = \frac{4\pi e}{\epsilon}(n + N_A z d),
\]
and integrating Eq. (4) twice with the boundary conditions (3),(6) yields the electrostatic potential,
\[
\phi(z) = \frac{1}{e}(E_c - E_{cs}) - \frac{4\pi e}{\epsilon}(n + N_A z d)z + \frac{2\pi e}{\epsilon} z^2 N_A +
\]
\[
\int_0^z dz' \int_0^{z'} \left[ \sum_{l,a,\alpha} n_{l,a,\alpha} \psi_{l,a,\alpha}^2(z'') \right] dz''.
\]
In turn, \( \phi(z) \) enters the mean-field one-dimensional Hamiltonian which determines the carrier motion in the directions perpendicular to the plane. At smaller densities, only the two valleys with larger mass \( m_\parallel \) corresponding to the \( z \)-axis motion are relevant (ladder number \( l = 0 \), valley degeneracy \( \gamma_0 = 2 \)), with the corresponding Hamiltonian
\[
\mathcal{H}_{0,\alpha} = E_c - \frac{\hbar^2}{2m_\parallel} \frac{\partial^2}{\partial z^2} - e\phi(z) + U \sum_{l,a} n_{l,a,\alpha} \psi_{l,a,\alpha}^2(z) - \frac{1}{2} \sigma_z \alpha \alpha,
\]
Here, \( H \) is the applied magnetic field in units of \( g\mu_B \) (bare \( g \)-factor times Bohr magnetone), and \( \sigma_z \) is the Pauli matrix. Owing to the finite thickness of Q2DEG, even an in-plane magnetic field leads to some orbital effects, as discussed elsewhere\[21,32\] (experimentally, orbital effects of the in-plane field are indeed seen in magnetotransport measurements at small densities\[6\]). These are expected to be minor and are omitted in the present treatment.

Eq. (8) includes the effects of short-range electron-electron interaction, Eq. (1). Presently, considerable research effort is directed at exploring the possibility of manipulating valley polarisation (“valleytronics”\[33\]). Here, however, we are concerned with the spin degree of freedom and for simplicity omit both the repulsion between same-spin electrons from different valleys, and the dependence of \( U \) on the valley indices. Yet we note that our approach can be easily generalised to include these effects.

As the densities increase, electrons begin to populate also the four valleys \( (l = 1, \gamma_1 = 4) \) where the larger mass \( m_\parallel \) corresponds to an in-plane direction of motion\[2\]. These are described by the Hamiltonian \( \mathcal{H}_{1,\alpha} \) which is given by Eq. (3) with the substitution \( m_\perp \rightarrow m_\parallel \) on the r. h. s. Since the electrostatic
potential confines the electrons to the vicinity of the surface, the relevant (low-energy) parts of the spectra of the Hamiltonians $H_{l,\alpha}$ are discrete, 

$$H_{l,\alpha}\psi_{l,a,\alpha} = E_{l,a,\alpha}\psi_{l,a,\alpha}.$$  

(9)

At $M = 0$ the levels are spin-degenerate ($E_{l,a,\uparrow} = E_{l,a,\downarrow}$), and form the two sequences (termed "ladders" in Ref. [31]) corresponding to $l = 0$ and $l = 1$. A spin-up electron at a level $l, a$ interacts with a spin-down electron with a level number $l', a'$ via a 2D contact repulsion,

$$U_{2D}^{l,a,l',a'} = U^{l,a,l',a'}_{2D} \delta(x-x')\delta(y-y'),$$

(10)

$$U_{2D}^{l,a,l',a'} = U \int_0^\infty \psi_{l,a,\uparrow}^2(z)\psi_{l',a',\downarrow}^2(z)dz.$$  

Note that while a similar integral with the same value of spin projection for both wave functions does not vanish, the same-spin electrons with different level indices do not interact. This is consistent with the underlying interaction $U_{2D}$ being a contact one, as the presence of two same-spin electrons at the same point is forbidden.

Within the mean-field scheme, both the Hartree field due to $U_{2D}$ and the self-consistent potential $\phi$ depend solely on $z$, hence the energy of a Q2DEG carrier is a sum of the corresponding eigenvalue $E_{a,\alpha}$ of the transverse-motion Hamiltonian and the free-particle contribution of the in-plane motion. In making this statement, we neglect the relativistic effects (spin-orbit coupling) which is justified not just because these are relatively small, but particularly because we are ultimately interested in thermodynamic quantities (magnetisation and susceptibility) which involve integrals over all directions of the in-plane momentum. The 2D carrier densities for given level and spin indices are thus given by

$$n_{l,a,\alpha} = -\gamma \nu_0 E_{l,a,\alpha} \theta(-E_{l,a,\alpha}),$$

$$\nu_0 = \frac{m_\perp}{2\pi \hbar^2}, \quad \nu_1 = \frac{\sqrt{m_\perp m_\parallel}}{2\pi \hbar^2},$$

(11)

(12)

where $m_\perp$ is the smaller effective mass and $\theta$ is the Heaviside function.

Throughout the relevant range of parameter values, the spread of the wave functions $\psi_{l,a,\alpha}(z)$ in the $z$ direction is several orders of magnitude smaller than the depletion layer width $z_d$. This means that the average values of $z$ for spin-up and -down carriers,

$$z_\alpha = \sum_{l,a} n_{l,a,\alpha} \int \psi_{l,a,\alpha}^2(z)dz/n_\alpha$$

(13)

are much smaller than $z_d$. Re-writing the last term in Eq. (7) as

$$\frac{4\pi e}{\epsilon} \sum_{l,a,\alpha} n_{l,a,\alpha} \left[ z \int_0^z \psi_{l,a,\alpha}^2(z')dz' - \int_0^z z'\psi_{l,a,\alpha}^2(z')dz' \right].$$

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Table 1 Typical values of system parameters and material properties as used in the calculations. \( m_e \) is the free electron mass. We chose the value of \( U \) corresponding to \( U_{\text{on-site}} \approx 3 \) eV.

| Quantity                        | Value               |
|---------------------------------|---------------------|
| SiO\(_2\) layer thickness       | \( d_{\text{ox}} \) 10\(^{-5}\) cm |
| Energy gap in Si                 | \( E_c \) 1.12 eV  |
| Transverse (larger) effective mass| \( m_l \) 0.916 \( m_e \) |
| In-plane (smaller) effective mass| \( m_\parallel \) 0.19 \( m_e \) |
| Acceptor density                | \( N_A \) 10\(^{15}\) cm\(^{-3}\) |
| Critical density of MIT         | \( n_c \) 7\cdot10\(^{10}\) cm\(^{-2}\) |
| 3D contact repulsion            | \( U \) 7.5\cdot10\(^{-34}\) erg\cdot cm\(^3\) |
| Dielectric constant of bulk Si  | \( \epsilon \) 11.9 |
| Dielectric constant of SiO\(_2\) | \( \epsilon_{\text{ox}} \) 3.9 |

we then find that the condition that \( \psi_{l,a,\alpha}(z) \) decays before the value of \( z \) reaches \( z_d \) translates into a useful relationship,

\[
\frac{2\pi e^2}{\epsilon} N_A z_d^2 = E_c - E_{cs} - \frac{4\pi e^2}{\epsilon} (n_\uparrow z_\uparrow + n_\downarrow z_\downarrow).
\]

(14)

In the following, we describe the results of calculations performed within this mean-field scheme in different regimes. The parameter values used are given in Table 1. In order to facilitate convergence of the numerical scheme, we made use of some of the algorithms employed previously in the non-interacting, zero-field case\([34]\). The \( z \)-coordinate is discretised, the system of Poisson and Schroedinger equations for \( z > 0 \) is solved, and its solution is fed back into the Hamiltonian for the next iteration. The infinite potential barrier at \( z \leq 0 \) is modelled by cutting off the hopping to the \( z = 0 \) point of the discretised \( z \)-axis from the \( z > 0 \) side.

In addition to including the effects of \( U \) and \( H \), an important difference from the previous calculations (including Ref. \([31]\)) is that instead of fixing \( E_{cs} \), we set the problem in a more precise way, fixing \( \phi_{\text{gate}} \) and solving for \( E_{cs}, n, M \) and \( z_d \). While the numerical calculations become more involved in this formulation of the problem, it corresponds to the actual measurement setup. Physically, the difference becomes apparent in the phenomenological treatment of the strongly-correlated case in Sect. 4 (where the bandwidth, and hence \( E_{cs} \), vary self-consistently), and also in the case of large magnetisation values encountered in Sects. 5 and 6.

Indeed, if at a fixed value of \( E_{cs} \) and at \( U = 0 \) the field \( H \) is increased beyond the value \( H_{1,a} \) corresponding to a full spin polarisation of carriers with a certain transverse-ladder and level indices \( l, a \), the value of \( n \) would begin to increase as \( \delta n = (H - H_{1,a})/(\gamma_{\nu} n) \) (the value of \( \partial H/\partial n \) would be renormalised in an interacting system). This is unphysical as in reality this variation of \( n \) is for the most part suppressed by the large capacitance \( C \) in Eq. 3. We find that the relative change in \( n \) is in fact rather small (see below, Sect. 6).

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\(^3\) In practice, we first fix \( E_{cs} \) and solve for \( n, M \) and \( z_d \), which can be done by feeding the results of each subsequent iteration back into the mean-field equations \([11]\) and \([13]\) (cf. Ref. \([24]\)); the appropriate value of \( E_{cs} \) is then found as the root of Eq. \([8]\).
Thus, the appropriate mean-field thermodynamic potential, which is min- 
imised by the suitable mean-field solution, corresponds to fixing $\phi_{gate}$, rather 
than $n$:

$$G = \sum_{l,a,\alpha} n_{l,a,\alpha} \left\{ E_{l,a,\alpha} + \frac{n_{l,a,\alpha}}{2\hbar v_l} + \frac{e}{2} \int_0^\infty \psi_{l,a,\alpha}^2(z) \phi(z) dz \right\} - 
- \sum_{l,l',a,a'} U_{l,a,l',a'} n_{l,a,\uparrow} n_{l',a,\downarrow} - \frac{e N_A}{2} \int_0^d \phi(z) dz 
- \frac{e}{2} (n + N_A z_d) \phi_{gate} .$$

(15)

The three terms in the first line are the energies of $z$-axis and in-plane motion 
of the Q2DEG carriers, and the correction to exclude the double-counting of 
their electrostatic energy. Double-counting of the interaction energy is cor-
rected by the first term in the second line, whereas the second term is the 
electrostatic energy of immobile electrons in the depletion layer. The last term, 
$-Q_{gate} \phi_{gate} / 2$, corresponds to our choosing $\phi_{gate}$ as an external variable.

A discussion of the applicability of our mean field scheme as outlined abo 
ve is relegated to the Appendix. We will now turn to the results obtained in 
different regimes.

3 Electrical quantum limit: the single-level solution

If the value of the gate voltage $\phi_{gate}$ is not too large, only the lowest quantum 
level $E_{0,0,\alpha}$ of the $z$-axis motion for each spin direction can lie below the 
chemical potential and be populated by the Q2DEG carriers:

$$n_{\alpha} = -2 \nu_{0} E_{0,0,\alpha} \theta(-E_{0,0,\alpha}) ,$$

$$n_{l,a,\alpha} = 0 \text{ for } a \geq 1 \text{ or } l \neq 0 .$$

(16)

This situation, which is termed electrical quantum limit, is somewhat simpler 
to analyse than the full multi-level case, and we will consider it first in order to 
illustrate certain key features of our mean-field results and underlying physical 
mechanisms. Moreover, we find it expedient to formally allow for values of 
$\phi_{gate}$ (or, equivalently, of $n$) to increase beyond the range where the electrical 
quantum limit is realised (the latter corresponds to lower carrier densities, 
$n \leq 3.2 \cdot 10^{12} \text{ cm}^{-2}$, see Sect. 5). This is accomplished by using Eq. (15) in 
place of Eq. (11), while keeping the rest of the mean field scheme intact. For 
quantitative results in the larger-density case of $n > 3.2 \cdot 10^{12} \text{ cm}^{-2}$, the reader 
should refer to Sect. 5 below. Since within the present section the ladder and 
level indices of all quantities are always equal to zero, we will suppress these.

Let us first briefly recall the usual Stoner picture, applicable both in the 
three-dimensional bulk and in the case of a perfectly 2D carriers. The latter have no 
$z$-axis degree of freedom and interact via contact potential, $U_{2D} = 
U_{2D} \delta(x-x') \delta(y-y')$. At the mean-field level, the effect of interaction is additive
with that of the applied field $H$, increasing the energy shifts of the two spin subbands (Zeeman splitting). The wave functions (which in the 2D case are given by products of $\delta(z)$ and the in-plane Bloch wave) are unaffected, and one readily finds the magnetic susceptibility, which in the 2D case is given by

$$\chi_0 = \frac{\nu_0}{1 - 2\nu_0 U_{2D}}. \quad (17)$$

As long as both the 2D density of states $\nu_0$ and $U_{2D}$ remain constant, $\chi_0$ does not depend on density. If either of these can be varied to the extent that the denominator of Eq. (17) vanishes, the ensuing divergence of $\chi_0$ suggests a ferromagnetic transition. Owing to the independence of $\nu_0$ on the carrier energy in the 2D case, this critical point has a peculiar character of a discontinuous transition with no hysteresis. Specifically, everywhere in the ferromagnetic phase the mean-field free energy minimum is attained in the fully spin-polarised state, whereas at the transition point itself the free energy does not depend on the magnetisation. Thus the magnetisation shows a jump at the transition point, simultaneous with vanishing of both the spin stiffness (from the ferromagnetic side) and inverse susceptibility.

These properties are strongly modified in the case of the Q2DEG as found in a Si inversion layer. First, note that the interaction strength $U_{2D}$ is given by Eq. (10) and depends on the density $n$. This is illustrated by the variational treatment, where the solution to Eq. (9) is sought in the form of an ansatz,

$$\psi_{\text{var}}(z) = \sqrt{b^3} z \exp(-bz/2), \quad (18)$$
yielding $U_{2D}^{\text{var}} = 3U b/16$. The value of $b$ is chosen by minimising the thermodynamic potential, Eq. (15), which yields

$$\frac{\hbar^2 b^3}{4m_{\parallel}} + \frac{3}{64} U n b^2 - \frac{12\pi e^2}{\epsilon} \left( N_A z_d + \frac{11}{32} n \right) = 0. \quad (19)$$

The difference from the $U = 0$ result of Ref. [31] is in the addition of the second term on the l. h. s. This results in a slight decrease of the value of $b$ (and hence in an increase of $z_0 \equiv z_{\uparrow} = z_{\downarrow} = 3/b$) in comparison to the non-interacting case. Similar to the $U = 0$ case, we find that the variational value of $E_0 = E_{\uparrow} = E_{\downarrow}$,

$$E_0 = E_{cs} + \frac{\hbar^2 b^2}{8m_{\parallel}} + \left( N_A z_d + \frac{11}{16} n \right) \frac{12\pi e^2}{eb} + \frac{3}{32} U n b, \quad (20)$$
closely approximates the numerical result.

In both $U = 0$ and $U > 0$ cases, the value of $b$ increases with increasing $n$. This is due to the increase of the ratio $n/N_A z_d$ ($z_d$ only weakly depends on $n$), which leads to a progressively larger part of the electrostatic field of the gate being screened by the mobile carriers within the layer of the Q2DEG (and not elsewhere within the depletion layer). Hence the potential $\phi(z)$ becomes steeper at small $z$, resulting in smaller $z_0$ and larger $b$ and $U_{2D}$.10
The decrease of $z_\alpha$ and increase of $U_{2D}$ are also found in the numerical solution of the mean-field equations in the paramagnetic state, i.e., below the critical density $n_1 \approx 8.4 \times 10^{13} \text{ cm}^{-2}$. The dependence of $U_{2D}$ and $z_\alpha$ on $n$ is depicted in Fig. 2, showing both variational and numerical results. We thus conclude that owing to the Q2DEG layer thinning, the quantity $\chi_0$ in the paramagnetic phase must be increasing with $n$, as indeed seen in numerical and variational results (see below, Figs. 4 and 5).

An additional effect arises in the interacting case, $U > 0$, with the result that the actual magnetic susceptibility $\chi = \partial M/\partial H$ is no longer given by Eq. (17). Indeed, it is easy to see that at $U > 0$, the appearance of a spin polarisation must be accompanied by a change in the transverse wave functions $\psi_\alpha(z)$ – a phenomenon which does not occur in the familiar Stoner picture as outlined above. At the level of our mean-field Hamiltonian, Eq. (5), the effect of interaction $U$ is that an electron feels an additional potential bump [the fourth term in Eq. (8)], centred around the peak of the opposite-spin wave function. In the absence of polarisation ($M = 0$), these peaks are located roughly at $z \sim z_0 = z_\uparrow = z_\downarrow$ and are identical for spin-up and -down carriers. When the magnetisation differs from zero (either spontaneously in the ferromagnetic phase or due to an applied magnetic field), the height (proportional to $n_\uparrow$) of the potential bump in the Hamiltonian $H_\downarrow$ of the spin-minority electrons increases, pushing these further away from $z_\uparrow$ in the direction of larger $z$ and increasing $z_\downarrow$ (note that now $z_\downarrow > z_\uparrow$, as seen in Fig. 2 for $n > n_1$). The associated bump in $H_\uparrow$ (although somewhat reduced in size, due to a reduction of $n_\downarrow$) is no longer centred at the peak of spin-majority electrons distribution – rather, it is “pushing” on these electrons from the side of larger $z$, leading to a reduction of $z_\uparrow$. This situation, which is shown schematically in Fig. 3, leads to decreasing the overlap between spin-up and spin-down wave-functions, hence to decreasing $U_{2D}$ [see Eq. (10)]. This behaviour of the numerical result for $U_{2D}$ is clearly reflected in Fig. 2 for $n > n_1$ (where $M > 0$, see the inset in Fig. 5 below). Ultimately the value of thermodynamic potential $G$ (Eq. (15)) is reduced in comparison with the case where no allowance is made for the change of $\psi_\alpha(z)$ with $M$. In other words, as a result of wave functions profile...
Fig. 3 Interaction-induced evolution of transverse-motion wave functions with increasing magnetisation $M$. The spin-up and -down wavefunctions at $M = 0$ coincide (unpolarised case, shown schematically by the dashed line). In the presence of interaction $U$, they split at $M > 0$ (solid lines). The electrostatic potential energy, $-e\phi(z)$, is shown for simplicity as a single dotted line [in reality, an increase of $M$ is accompanied by a small self-consistent change in $\phi(z)$ and in the value of $z_d$].

change it costs less energy to form a non-zero magnetisation, which translates into an increased value of susceptibility $\chi$ and into a decreased critical value of the interaction $U_{2D}(n)$ (evaluated at $M = 0$), required to destabilise the paramagnetic state.\textsuperscript{4} In the purely 2D case, the latter is determined by a condition [cf. Eq. (17)]

$$1 - 2n_0U_{2D} = 0,$$

(21)

known as the Stoner criterion. As we already mentioned, what is varied in the actual measurements is the gate voltage $\phi_{\text{gate}}$, which in turn causes the variation of $n$, directly accessible by measuring the Hall voltage. Hence the relevant quantity is the value of $n$, corresponding to the ferromagnetic transition. Owing to the dependence of $U_{2D}$ on $n$, the l. h. s. of Eq. (21) for a given $U$ may vanish at a certain critical value density, $n_0$ (which is either very large or even infinite for our values of parameters). In reality, we find that the Stoner criterion is relaxed, viz., the l. h. s. of Eq. (21), is still positive at the critical density, $n = n_1$. This is due to self-consistent dependence of the transverse-motion wave functions on magnetisation $M$, as discussed above.

These ideas can be illustrated with the help of variational wave functions. As explained above, using the wave function (18) leads to

$$\chi^{\var}_0 = \frac{\nu_0}{1 - 3U(n)\nu_0/8}, \quad 1 - 3U(n)\nu_0/8 = 0,$$

(22)

where $n_0^{\var}$ is the corresponding critical density. Let us now allow the spin-up and -down wave functions to differ form each other at $M \neq 0$, by writing, instead of Eq. (18),

$$\psi_\alpha(z) = \sqrt{b_\alpha^2/2} \exp(-b_\alpha z/2).$$

(23)

Here, we are interested in the limit of small polarisation, $M \ll n$. Thus, $b_{\uparrow, \downarrow} - b = \pm b_1$ is a small spin-dependent correction to the value of $b$ which solves Eq. (19) at $M = 0$ and $H = 0$. We then substitute Eq. (23) into Eq. (15), which includes re-calculating the variational energies $E_\alpha = \int_0^\infty \psi_\alpha(z)H_\alpha \psi_\alpha(z)dz$. To

\textsuperscript{4} Note that this wave functions change is not restricted to electrons in the vicinity of the 2D Fermi surface. This implies that Fermi liquid theory cannot be used to evaluate magnetic susceptibility, and the conventional Fermi-liquid expression for $\chi$, which can be viewed as an analogue of Eq. (17), is inapplicable in this case.
leading-order in $b_1$, $M$, and $H$, the thermodynamic potential $G$ acquires a correction,

\[
\delta G = \left\{ \frac{\hbar^2 n}{8m} + \left(12N_A z_d + \frac{21}{16} n \right) \frac{\pi e^2 n}{eb} + \frac{9U n^2}{64b} + \frac{9}{2048} \nu_0 U^2 n^2 \right\} b_1^2 - \left(1 - \frac{3}{8} \nu_0 bU \right) \left\{ \frac{3}{32} U n M b_1 + \frac{3}{16} U b M^2 + MH \right\} + \frac{3}{32} U n \nu_0 b_1 H + \frac{1}{2} \nu_0 H^2.
\]

(24)

Note that $b_1$, $H$, and the magnetisation $M = (n_\uparrow - n_\downarrow)/2$ are not mutually independent. Indeed, $M$ is obviously determined by the first-order correction to the variational energy $E_0$,

\[
M = -\nu_0 (E_\uparrow - E_\downarrow) = \nu_0 H + \frac{3}{8} \nu_0 U b M - \left\{ \frac{\hbar^2 b}{4m} - \left( N_A z_d + \frac{11}{32} n \right) \frac{12\pi e^2}{eb} \right\} 2\nu b_1,
\]

(25)

or, with the help of Eq. (19),

\[
\left(1 - \frac{3}{8} \nu_0 bU \right) M - \left( \frac{3}{32} U n \nu_0 b + \nu_0 H \right) = 0.
\]

(26)

We can now use this to exclude $b_1$ in Eq. (24). Minimising $\delta G$ with respect to $M$ then yields $M = \chi^{var} H$, with the corresponding susceptibility

\[
\chi^{var} = \frac{\nu_0}{1 - 3U b(n)\nu_0/8 - L},
\]

(27)

\[
L = \frac{9\nu_0 U^2 n b}{2048} \left\{ \frac{\hbar^2 b^2}{8m} + \left( N_a z_d + \frac{7}{64} n \right) \frac{12\pi e^2}{eb} - \frac{9}{64} U n b \right\}^{-1}.
\]

(28)

We see that the effect of wave function changing with $M$ gives rise to the last term in the denominator in Eq. (27) [cf. Eq. (22)], and therefore leads to the susceptibility increase. The second term in the denominator equals $2\nu_0 U^{var}$, and the ratio $L/(2\nu_0 U^{var})$ is roughly of the order of $nU_{2D}/(E_0 - E_{cs})$. Here, $nU_{2D}/2$ is the net scale of the energy of the contact interaction, whereas $E_0 - E_{cs}$ is the energy of quantised motion along the $z$-axis [see Eq. (20)].

These variational results are illustrated in Fig. 4, where the solid line represents Eq. (22), which uses the ansatz for the wave function and does not allow for a wave function change with increasing $M$. The variational susceptibility $\chi^{var}_0$ slowly increases with $n$ from the non-interacting value of $\chi^{var}_0 = \nu_0$, reflecting the increase of $U_{2D}$ as discussed above. Within a very broad range of $n$, it does not show any critical behaviour; indeed, at $n$ as large as $3.5 \times 10^{14}$ cm$^{-2}$, $\chi^{var}_0/\nu_0$ reaches the value of only 1.6. On the other hand, the quantity
\( \chi_{\text{var}} \) [dashed line; see Eq. (27)] deviates upwards from \( \chi_{\text{var}}^0 \) and diverges at \( n_{\text{var}} \approx 1.13 \cdot 10^{14} \text{ cm}^{-2} \), suggesting a ferromagnetic transition. This is a consequence of the polarisation dependence of the wavefunctions (23), as outlined above. We note that the difference between \( \chi_{\text{var}} \) and \( \chi_{\text{var}}^0 \) becomes appreciable only at large densities \( n \), and the critical value \( n_{\text{var}} \) is also very large. This is due to our chosen wave functions shape, Eq. (23). Indeed, it is clear that the way these wave functions are changed with \( H \) is far from optimal. Much lower result for the critical density (\( \tilde{n}_{\text{var}} \approx 2.89 \cdot 10^{13} \text{ cm}^{-2} \)) is obtained when using an ansatz which includes additional parameters \( \kappa_{\uparrow, \downarrow} \):

\[
\bar{\psi}_\alpha(z) \propto z \sqrt{1 + \kappa_\alpha b_\alpha^2 z^2} \exp(-b_\alpha z/2).
\]

This results in a somewhat cumbersome expression for susceptibility, which is given in Ref. [30]; in Fig. 4 the corresponding value is plotted with a dotted line. It does not merge with \( \chi_{\text{var}}^0 \) even at low densities because the optimal value of coefficient \( \kappa_{\uparrow} = \kappa_{\downarrow} \) at \( M = 0 \) differs from zero[30].

The numerical solution of the mean-field equations in the single-level case yields the solid line in Fig. 5 (for comparison, the dashed line shows the value of \( \chi_{\text{var}} \)). The numerical result shows critical behaviour, with the corresponding critical \( n_1 \) in the interval between \( n_{\text{var}} \) and \( n_{\text{var}} \). Thus, we conclude that the latter two variational approximations respectively overestimate and underestimate the ferromagnetic tendencies. The importance of the wave-function change with \( M \) in case of numerical results is illustrated by the dotted line in Fig. 5 which shows the value of \( \chi_0 \), Eq. (17), computed using the numerically calculated value of \( U_{2D} \) at \( M = 0 \) [see Eq. (10) and Fig. 2]. In other words, when calculating \( \chi_0 \) we used the exact mean field wave functions for \( M = 0 \). Thus, the quantity \( \chi_0 \) is defined only at \( n < n_1 \), and we see that it remains smaller than the actual susceptibility \( \chi \) and does not show any tendency toward criticality (similarly to \( \chi_{\text{var}}^0 \) in Fig. 4). The interaction energy per a Q2DEG carrier can be estimated as \( nU_{2D}/2 \) [see Eq. (8)] and decreases with \( n \). Hence at small \( n \) it eventually becomes much smaller than the energy.
The density dependence of magnetisation \( M \) in the ferromagnetic phase at \( n > n_1 \) is shown in the inset of Fig. 5. It looks reminiscent of a typical mean field behaviour of an order parameter, yet as explained above this is not what is found in the Stoner treatment of a purely 2D case, where a jump in \( M \) is obtained. The difference is due to the transverse wave functions changing with increasing \( M \): the resultant decrease of \( U_{2D} \) moderates the increase of \( M \) with density.

In the preliminary publication [30], we used a larger value of \( U \) (4/3 of the value used presently), leading to smaller values of numerical and variational critical densities. We find that the result of Ref. [30] for the numerical solution equals 0.64 of our present \( n_1 \), and similarly for the variational ansatz, Eq. (29). Ref. [30] yields the critical density of 0.66\( \tilde{n}_{\text{var}} \). We conclude that critical density is strongly dependent on \( U \).

As already mentioned, the simplified treatment described in this section, while illuminating, does not apply in the two important limiting cases, viz., the metallic behaviour at high densities and the correlated regime immediately above the MIT. We will now consider these in more detail.

### 4 Low carrier densities above the MIT

Within the simplified single-level treatment of Sect. 3, the obtained value of magnetic susceptibility was found to increase with increasing density \( n \), eventually reaching a ferromagnetic instability deep in the high-density region (see
Figs. 4 and 5). We note that at the low densities above the MIT, only the lowest transverse-motion level lies below the chemical potential, hence Eq. (16), used in Sect. 3, is certainly valid. In this low-density range, the computed value of susceptibility as plotted in Fig. 5 (solid line) only slightly deviates from the non-interacting result, \( \chi \equiv \nu_0 \) (see the dashed-dotted line in Fig. 6 below). However, the approach used in Sect. 3 is contingent upon the validity of the assumption that after taking into account both Coulomb and contact interactions on average, the in-plane carrier motion can be treated as free. The latter becomes invalid at low densities, where the dimensionless parameter \( r_s = m_\perp e^2/(\hbar^2 \sqrt{\pi n}) \) (relative strength of the long-range Coulomb interaction) significantly exceeds 1. Since at \( n \approx n_c = 7\cdot10^{10} \text{ cm}^{-2} \) (see Table 1) we find \( r_s \approx 6.4 \), our mean field scheme as outlined in Sect. 2 is indeed inapplicable in this region. Here, we wish to argue that a phenomenologically-motivated modification should be introduced in the self-consistent mean field scheme in this regime.

Recently, it has been noted [22] that the available data for the effective mass, susceptibility, and saturation field value in Si-MOSFETs above the MIT can be described phenomenologically by a 2D non-interacting Fermi gas with a renormalised in-plane mass:

\[
\tilde{m}_\perp = m_\perp \frac{n}{n - n_c} .
\]  

(30)

This behaviour was anticipated theoretically [36], and discussed in the general context of metal-insulator transitions [37]. Similar results were also obtained by radiative spectra measurements on GaAs/AlGaAs heterostructures [38]. In addition, higher-temperature entropy measurements [39] on a Si-MOSFET sample yield an effective mass peak at low densities. The peak becomes more pronounced when the temperature is lowered, and this effective mass enhancement is in a qualitative agreement with the low-temperature results as described by Eq. (30). The latter equation leads to a renormalisation of the density of states,

\[
\tilde{\nu} \equiv \frac{\tilde{m}_\perp}{2\pi \hbar^2} = \frac{n}{n - n_c} \nu_0
\]  

(31)

and (in the absence of the short-range interaction \( U \)) to the Pauli in-plane susceptibility [22],

\[
\chi_P = \tilde{\nu} ,
\]  

(32)

which diverges at the MIT (at \( n = n_c \)). The latter is due to the effective band narrowing, and does not necessarily imply a magnetic instability (in agreement also with Ref. [13]).

In the low-density region of \( n \lesssim 10^{11} \text{ cm}^{-2} \), the average distance between carriers is large in comparison with the inversion layer thickness (of the order of \( 10^{-6} \text{ cm} \)). It is then natural to expect that while the long-range correlations are in fact prominent (as indicated by large values of \( r_s \)), they affect the in-plane motion of the carriers only, whereas the finite carrier motion along the \( z \)-axis is still determined by a nearly triangular self-consistent potential \( \phi(z) \).
Hence it appears that the effects of an additional short-range interaction $U$ can be probed within the Hartree scheme as before. The only modification which needs to be introduced in the mean-field scheme of Sect. \ref{sec:mean-field} is the substitution of $\tilde{\nu}$ in place of $\nu_0$ in Eq. (11) [or equivalently in Eq. (16)]. We emphasise that this approach does not constitute a self-contained theoretical treatment (hitherto missing), which should include both interactions from the start. In reality, what we attempt here is a phenomenological estimate, whose results underline the necessity of constructing a proper theoretical description.

When neglecting the wave function dependence on magnetisation (which is indeed justified in this regime, see below), we obtain instead of Eq. (17):

$$\chi_0 = \frac{\tilde{\nu}}{1 - 2\tilde{\nu}U_{2D}}. \quad (33)$$

As the density is lowered toward $n_c$, the value of $U_{2D}$ stays finite while $\tilde{\nu}$ diverges, signalling a ferromagnetic instability at

$$n_* = n_c (1 + 2\nu_0 U_{2D}) . \quad (34)$$

In order to roughly estimate the difference between this transition and the MIT, one can again use the variational ansatz \cite{ref:var}, which yields $U_{2D}^{var} = 3U/b/16$. The second term in Eq. (19) for the variational parameter $b$ is now negligible, whereas in other terms $n$ and $N_A z_d$ are of the same order of magnitude as $n_c$. Omitting all factors of order of unity, we obtain an order-of-magnitude estimate,

$$n_* - n_c \sim U\nu_0 n_c^{3/2} r_1^{1/3} . \quad (35)$$

Variational and numerical results for susceptibility are shown in Fig. 6. As explained above, at $U = 0$ the (Pauli) susceptibility $\chi_P$, Eq. (32), diverges at $n = n_c$ but does not show any ferromagnetic singularity at $n > n_c$ (dashed line in Fig. 6). Numerical solution of the mean-field equations [with renormalised density of states $\tilde{\nu}$, see Eq. (31)] yields the value of $\chi$ showed by the solid line, with a ferromagnetic instability at $n_* \approx 7.43 \cdot 10^{10}$ cm$^{-2}$. Hence taking into account the short-range $U$ brings about the ferromagnetic transition above the MIT. The dashed-dotted line shows the results obtained within the approach of Sect. \ref{sec:3d} with the same value of $U$ but without renormalising the density of states (i.e., using $\nu_0$ rather than $\tilde{\nu}$). While the dashed-dotted and solid lines eventually merge at higher $n$ (where the effects of long-range correlations are weak), the dashed-dotted line remains featureless all the way down to $n = n_c$.

Similar to Sect. \ref{sec:3d} above, a comparison with the results of Ref. \cite{ref:3d} allows to verify the dependence of $n_*$ on $U$. We find that the result of Ref. \cite{ref:3d} for $(n_* - n_c)/n_c$ is about 1.3 times larger than the one obtained herein, roughly agreeing with Eq. (35).

We note that on the scale of the plot, the numerical value of $\chi(n)$ (solid line in Fig. 6) is indistinguishable from $\chi_0$, Eq. (33). This is because in the low-density regime, the characteristic energy scale $n U_{2D}$ of the short-range interaction is much smaller than the ground-state energy $E_0 - E_{cs}$ of the transverse carrier motion (the latter is about 16 meV at $n = n_*$ and increases
to $E_0 - E_{cs} \approx 47$ meV at $n = 10^{12}$ cm$^{-2}$, whereas $nU_{2D}$ increases from 0.05 meV to about 1 meV. In this regime, the short-range $U$ almost does not perturb the transverse motion, and in particular the magnetisation dependence of the carrier wave functions (see Fig. 6) is very weak. In turn, this magnetisation dependence of $\psi_\alpha(z)$ is the only ingredient that distinguishes the full numerical solution of mean-field equations from the “Stoner” approach which yields Eq. (33).

The dotted line in Fig. 6 corresponds to using the ansatz, Eq. (18), for $\psi_\alpha(z)$, which amounts to substituting $U_{2D}^{var}$ for $U_{2D}$ in Eq. (33). This would slightly underestimate the value of density at the ferromagnetic transition, the discrepancy being due to the variational nature of this approach.

The ferromagnetic transition is second-order, and the full polarisation is reached at a certain density $n_F < n_\ast$. Numerically, we find that the transition is very steep, with $n_\ast - n_F \sim 5 \cdot 10^7$ cm$^{-2}$. The latter value presumably is well below any experimental accuracy. This is in line with the preceding discussion: as explained in Sect. 5 above, within the conventional Stoner approach the mean-field transition would have been perfectly abrupt. The fact that the transition is in fact smooth is due to the dependence of wave functions on $M$ (Fig. 6), which is very weak at low densities. Indeed, in the fully polarised state below $n_F$ we find $\langle z_\uparrow - z_\downarrow \rangle / (z_\uparrow + z_\downarrow) \approx 6 \cdot 10^{-4}$, reflecting a rather minute difference in the profile of spin-up and spin-down distributions. This should be contrasted with a pronounced difference between $z_\uparrow$ and $z_\downarrow$ above the high-density magnetic transition, as seen in Fig. 6.

We emphasise that this mean field picture may be significantly modified once the effects of fluctuations are taken into account. These may increase the value of $n_\ast - n_c$ and turn the transition first-order; the latter would be in line with reported inhomogeneous behaviour in this region.

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5 Here $n_\downarrow = 0$, and we need to re-define $z_\downarrow$ as $z_\downarrow = \int \psi_0^2(z) zdz$ [cf Eq. (13)].
The effects of finite temperature (beyond the strictly degenerate regime) are outside the scope of the present article. We speculate that the peak (rather than a divergence) of the effective mass reported in Ref. [39] may correspond to the scenario whereby the ferromagnetic ordering is stabilised at temperatures below those used in Ref. [39].

Our tentative results as outlined above imply that a ferromagnetic transition occurs at a critical value of density \( n^* \) which is a few per cent larger than that of the MIT \( n_c \). On the other hand, available experimental results suggest the following two scenarios: (i) As the density is decreased toward the MIT, the susceptibility increases, reaching a large but finite value at the point of MIT [11]. Then the (asymptotic) value of transition critical density \( n_c \) would lie below \( n_c \) (the ferromagnetic transition is preempted by the MIT, at which point the properties of the system change and there is no transition at \( n = n_* \)). (ii) The susceptibility actually diverges in the vicinity of the MIT, with the two transitions occurring simultaneously or very close to each other [4]. While it might appear that our present conclusions do not support either of these two possibilities, we wish to argue that our results can be re-interpreted and reconciled with the second one.

Once the system is fully spin-polarised by an applied field, it exhibits insulating behaviour even at densities above the \( H = 0 \) MIT point [4]. The in-plane field can affect transport properties only via spin, i.e. via the magnetisation \( M \) (or equivalently via the degree of spin polarisation). Thus, it seems logical to expect that whenever the system is fully spin-polarised (either due to an external field or to intrinsic ferromagnetism), it turns insulating. That would mean that the actual MIT takes place at \( n = n_* \) (we recall that the width of magnetic transition is expected to be negligible), whereas \( n_c \) (which is a few percentage points below \( n_* \)) retains the meaning of an extrapolation parameter controlling the bandwidth renormalisation [see Eqs. (30–31)]. We note that the latter is somewhat similar to the scenario discussed in Ref. [18] in the context of long-range Coulomb interaction alone.

The available experimental data for the effective mass (which can be deduced, e.g., from the transport measurements [42]) and susceptibility do not allow to conclude with certainty that the latter indeed follows either Eq. (33), and not Eq. (32). The observed systematic differences [8, 9, 22] [see, e.g., Fig. 9 in Ref. [8]] between the measured \( \chi \) and the calculated Pauli value \( \chi_P \) [Eq. (32)] may be due, at least in part, to the experimental issues or inaccuracies of interpretation. In order to reliably verify the importance of short-range interaction, further measurements would need to be performed closer to the MIT.

---

6 In addition to susceptibility measurements, further support comes from the density dependence of magnetic field value required to fully spin-polarise the system [40, 41].
5 The high-density metallic regime

When the density is increasing further away from the MIT, the susceptibility continues to decrease, as shown by the solid line in Fig. 7 (which is a continuation of the solid line in Fig. 6). This is due to the decreasing influence of the long-range correlations [taken into account phenomenologically via Eq. (30)], and indeed reflects the decreasing $U = 0$ phenomenological susceptibility [Pauli susceptibility, Eq. (32)], dashed line in Figs. 6 and 7. Qualitative estimate confirms that in this region the long-range correlations weaken and ultimately cease to dominate, with $r_s \approx 1$ at $n = 3 \cdot 10^{12} \text{cm}^{-2}$. It is seen that as the value of $n$ continues to increase, the susceptibility passes through a broad minimum at $n \approx 2.4 \cdot 10^{12} \text{cm}^{-2}$ and begins to increase. The latter feature is due to the increasing role of the contact interaction $U$. This corresponds to the increase shown by the dashed-dotted line, which depicts the value of susceptibility calculated using the unrenormalised value $\nu_0$ [see Eq. (12)] of the density of states (i.e., shows the effects of $U$ only, along the lines of Sect. 3).

A further increase in $n$ leads to populating the second (first excited) level of carrier motion in the $z$ direction. Indeed, we already mentioned in Sect. 3 that modelling the behaviour of the system at higher inversion-level carrier densities $n$ requires taking into account the presence of multiple occupied levels. Thus, one has to implement the complete mean field scheme, without a simplification utilised in Sects. 3 and 4 where we used Eq. (16) in place of a more general Eq. (11). On the other hand, at these larger values of $n$ the phenomenological carrier density of states $\tilde{\nu}$ [see Eq. (31)] approaches its unrenormalised value $\nu_0$. Indeed, the effect of the mass renormalisation at $n = 3 \cdot 10^{12} \text{cm}^{-2}$ on susceptibility is already negligible (the difference between solid and dashed-dotted lines at the right edge of Fig. 7), and decreases further with increasing $n$. Thus, we cross into the normal Fermi liquid regime, and we may use the unrenormalised value $\nu_0$ of the density of states (which somewhat simplifies
the complicated numerical calculation). A possibility of strong Fermi-liquid renormalisations at larger $n$ owing to the contact interaction $U$ will be discussed in Sect. 7. Given the absence of data for high densities, we will be using the unrenormalised value $\nu_0$ throughout.

We again begin with the conventional Stoner mean-field description of the paramagnetic phase, assuming that the transverse wave functions $\psi_{l,a,\alpha}(z)$ do not change when the magnetisation $M$ varies. The latter assumption is essentially a variational one, and implies that when $M$ is small, the $(l,a)$th transverse energy level of a spin-up electron (which at $M = 0$ is given by $E_{l,a,\uparrow}$) acquires a correction,

$$
\delta^{(0)}E_{l,a,\uparrow} = \sum_{l',a'} U_{l,a,l',a'}^{2D} \delta^{(0)}n_{l',a',\downarrow} - \frac{1}{2}H,
$$

and similarly for spin-down electrons. The matrix $U_{2D}$ (which in the paramagnetic phase is symmetric) is defined by Eq. (10), and the corrections $\delta^{(0)}n_{l,a,a}$ to the level occupancies at $M \neq 0$ are found self-consistently from Eq. (11). This leads to a set of self-consistency equations,

$$
\delta^{(0)}n_{l,a,\uparrow} - \delta^{(0)}n_{l,a,\downarrow} = \gamma \nu_l \times
$$

$$
\times \left[ H + \sum_{l',a'} U_{l,a,l',a'}^{2D} \left( \delta^{(0)}n_{l',a',\uparrow} - \delta^{(0)}n_{l',a',\downarrow} \right) \right].
$$

This linear system is readily solved, and the “Stoner” susceptibility is then found as

$$
\chi_0 = \frac{1}{2H} \sum_{a} \left( \delta^{(0)}n_{a,\uparrow} - \delta^{(0)}n_{a,\downarrow} \right).
$$

In the single-level case, Eq. (38) yields the familiar single-level result, Eq. (17). On the other hand, we note that in the multi-level case the “Stoner” result (38) includes effects of the restricted geometry, not found in either 3D bulk or purely 2D systems (see below).

As long as the carrier density is not too high, $n \lesssim 3 \cdot 10^{13}$ cm$^{-2}$, the susceptibility value obtained by numerically solving the mean field equations (solid line in Fig. 8) is well described by the Stoner theory [dotted line, obtained from Eq. (38)]. As expected already in the non-interacting case ($U = 0$, corresponding to the dashed-dotted line in Fig. 8), once a new transverse motion level is populated the susceptibility suffers a jump. For our values of parameters we find that these are located at $n_{(0,1)} \approx 3.3 \cdot 10^{12}$ cm$^{-2}$ and $n_{(1,0)} \approx 4.9 \cdot 10^{12}$ cm$^{-2}$ (where the superscript is the number of the transverse motion level which dips below the Fermi level at the corresponding value of $n$, preceded by the number of the corresponding ladder). We note that the magnitude of the steps in $\chi/\nu_0$ is renormalised in comparison with the non-interacting case, where for a step at every $n = n_{(l,a)}$ we find $\delta\chi^{(l,a)} = \gamma \nu_l / 2$. For example, the magnitude of the step at $n = n_{(0,1)}$ in our case is $\delta\chi/\nu_0 \approx 1.08$. As readily seen with the help of Eq. (38), the difference from unity is due to
the non-zero matrix elements $U_{2D}^{10,10,1} = U_{2D}^{10,10,0} (\approx 2.7 \cdot 10^{-28} \text{erg} \cdot \text{cm}^2)$ and $U_{2D}^{10,10,1} (\approx 9.9 \cdot 10^{-28} \text{erg} \cdot \text{cm}^2)$. On the other hand, the difference of the baseline value of $\chi/\nu_0$ just below the step, $\chi/\nu_0 \approx 1.12$, from unity is due to the (larger) $U_{2D}^{10,10,0} (\approx 2.2 \cdot 10^{-27} \text{erg} \cdot \text{cm}^2)$. Note that in this density range, the values of $U_{2D}^{l,l',a'}$ at fixed $n$ are approximately proportional to $U$.

At $n \approx n^{(0,1)}$, the magnetic susceptibility $\chi$ deviates only slightly from its value in the non-interacting case (see the dashed-dotted line in Fig. 8), confirming that the effects of short-range interaction are relatively weak. Thus it is natural that the precise value of $n^{(1,0)}$ does not strongly depend on $U$, e.g., at $U = 0$ we get $n^{(0,1)} = 3.6 \cdot 10^{12} \text{cm}^{-2}$. On the other hand, $n^{(0,1)}$ is sensitive to the acceptor density $N_A$ which can vary broadly. Indeed, for $U = 0$ and $N_A = 10^{14} \text{cm}^{-3}$ we find $n^{(0,1)} \approx 2.2 \cdot 10^{12} \text{cm}^{-2}$ (which again agrees with Ref. [31]), whereas for $U = 0$ and $N_A = 10^{16} \text{cm}^{-3}$, $n^{(0,1)} \approx 6.1 \cdot 10^{12} \text{cm}^{-2}$.

With a further increase in density, the numerical results for $\chi$ in Fig. 8 begin to deviate from the Stoner susceptibility $\chi_0$. This is because the short-range interaction begins to affect the transverse carrier motion, and the wave functions become polarisation dependent (see Fig. 3). Indeed, at $n = 3 \cdot 10^{13} \text{cm}^{-2}$ the most important energy scale of the transverse motion, $E_{0,0,a} - E_{cs} \approx 480 \text{meV}$, is only a few times larger than the (roughly estimated) interaction energy scale, $2\nu_{0,0}U_{2D}^{00,00,0} \approx 70 \text{meV}$ (see discussion in Sect. 3 above).

This deviation of $\chi$ from $\chi_0$ further increases with $n$, until $\chi(n)$ becomes critical signalling a second-order ferromagnetic phase transition at $n_{FM} \approx 1.15 \cdot 10^{14} \text{cm}^{-2}$. As mentioned above, at this point carriers populate three spin-degenerate levels of the $z$-axis motion, which is the reason behind the increase in the critical density $n_{FM}$ in comparison to the single-level estimate $n_1$ of Sect. 3. Indeed, the wavefunction of higher levels are broader in the $z$-direction, which results in smaller values of the corresponding $U_{2D}^{l,l'}$ (see the data for $n = n^{(0,1)}$ above) and hence in a certain weakening of the interaction effects.
Overall, the dotted line in Fig. 8, which shows the multi-band Stoner susceptibility $\chi_0$, Eq. (38), follows the numerical result much more closely than in the single-level case of Sect. 3 (see Fig. 5). The reason is that, as mentioned above, the respective transverse wavefunction spreads differ for different active levels. Within the multi-level Stoner scheme, at $H \neq 0$ these levels are shifted in a non-uniform self-consistent fashion [see Eq. (36)], giving rise to an $H$-dependent difference in the profile of the net spin-down and spin-up charge densities (cf. Fig. 3). In this way, a Stoner treatment yielding Eq. (38) is able, in the multi-level case only, to partially mimic the effect of wavefunction change as captured by the full numerical solution of the mean field equations, resulting in a better fit.

Still, we find that Eq. (38) predicts a (discontinuous) ferromagnetic transition at $n_0 \approx 1.47 \cdot 10^{14} \text{ cm}^{-2}$, well above the actual transition density $n_{FM}$. Hence the adequate self-consistent treatment of the wave function dependence on $M$ is important for evaluating the critical density. In a direct analogy with Sect. 3, we conclude that the Stoner criterion of ferromagnetism is relaxed.

Density dependence of the spontaneous magnetisation, $M(n)$, is shown in Fig. 9 (solid line). The fact that the transition at $n = n_{FM}$ is smooth is explained (as in Sect. 3 see also Sect. 6) by the magnetisation dependence of the $z$-axis motion wavefunctions. This effect is surprisingly strong: an increase of $n$ by a factor of 2.8 is required to saturate the relative magnetisation. Interestingly, the value of $2M/n$ then reaches a plateau at about 0.98 (with the 0th spin-down levels in both ladders pinned just below the Fermi energy). The complete spin polarisation, $M = n/2$, is not attained even at $n \sim 2.3 \cdot 10^{15} \text{ cm}^{-2}$. Given the inversion layer thickness of the order of $10^{-7} \text{ cm}$, this value approaches the normal-metal range of three-dimensional carrier densities, where our approach becomes invalid.

Owing to a larger effective mass and higher valley degeneracy, the only active level (0th) in the 1st ladder provides most of the density of states at the Fermi level. The evolution of average $z$ values of carriers in this level,

$$z_{\alpha}^{(1,0)} = \int \psi_{1,0,\alpha}^2(z)dz,$$

with $M$, is characterised by increasing ratio

$$p^{(1,0)} = \frac{z_{\downarrow}^{(1,0)} - z_{\uparrow}^{(1,0)}}{z_{\downarrow}^{(1,0)} + z_{\uparrow}^{(1,0)}}$$ (39)

(dashed line in Fig 9). Clearly, the spatial separation between opposite-spin carriers belonging to this level increases with magnetisation, and the magnitude of $p^{(1,0)}$ mirrors the value of $M$. This can be understood in terms of Fig. 3 (see discussion in Sect. 3).

Values of $\chi_{M=0}^{l,l'}$, needed to evaluate $\chi_0$ in the region $n_{FM} < n < n_0$, are obtained by finding the $\bar{M} = 0$ (spin-degenerate) solution to the mean field equations, even as this solution does not minimise the thermodynamic potential, Eq. (15).
On the other hand, the behaviour of overall average values $z_\alpha$ (including contributions from all active levels, see Eq. (15)) is complicated by effects of particle re-distribution between different levels, as well as by inter-level interaction. For example, as $M$ increases, a larger fraction of minority carriers resides in the levels of the 0th ladder which may reduce the ratio

$$p = \frac{z_{\downarrow} - z_{\uparrow}}{z_{\downarrow} + z_{\uparrow}}$$

(see the dotted line in Fig. 9).

In the ferromagnetic phase, spin-up and spin-down carriers no longer begin to populate new $z$-axis motion levels simultaneously. Indeed, our result for $\chi(n)$ shows further upward steps at $n_{\uparrow}^{(0,2)} \approx 1.64 \cdot 10^{14}$ cm$^{-2}$, $n_{\uparrow}^{(0,3)} \approx 2.83 \cdot 10^{14}$ cm$^{-2}$, and $n_{\uparrow}^{(1,1)} \approx 3.91 \cdot 10^{14}$ cm$^{-2}$, where spin-up electrons (only) begin to populate the 2nd and 3rd excited levels in the 0th ladder and the 1st excited level in the 1st ladder, respectively. In addition, there is a downward step at $\tilde{n}_{\downarrow}^{(0,1)} \approx 3.23 \cdot 10^{14}$ cm$^{-2}$, where due to increasing polarisation $M(n)$, the spin-down electrons cease to populate the 1st excited level in the 0th ladder. Interestingly, these points do not correspond to any noticeable features of magnetisation, $M(n)$ (see Fig. 9). Overall, the non-monotonous density dependence of $\chi(n)$ in Fig. 8 in the ferromagnetic region above $n_{FM}$ should be ascribed to a combined effect of the wave functions changing and the carriers redistributing between the bands with increasing $M$.

While relegating further discussion of these results to Sect. 7, we note that solving the mean-field equations in the multilevel case, in a broad range of values of density $n$, is a delicate numerical problem. For a given value of $E_{cs}$, the mean field equations (see Sect. 2) are first solved for a suitable variational ansatz of the type (15), yielding the values of $z_{d}$, $n$, and $M$ and the corrected wave functions; these are then fed back into the mean field equations and the process repeated until convergence is achieved (cf. Ref. [34]). It is found that the value of $M$ converges rather slowly (as opposed to $n$ and $z_d$), necessitating a large number of iterations (up to some 8400 near the critical point, $n = n_{FM}$).

In addition, since the wave function spread in the $z$-direction increases for higher levels, particular care should be taken in choosing large-$z$ cutoff $z_{max}$.
when solving the Schrödinger equation \( \text{(9)} \) and evaluating required integrals.

For the values of \( n \) shown in Fig. 8, we found it necessary to increase the ratio of \( z_{\text{max}} \) to the average carrier coordinate \((z_{\uparrow}n_{\uparrow} + z_{\downarrow}n_{\downarrow})/n\) in stages from 7 for smaller \( n \) to 34 for largest values. This subtlety, as well as the important role played by the \( l = 1 \) ladder of energy levels, was overlooked in Ref. [30], hence the preliminary results for the high-density regime reported therein are quantitatively incorrect.

### 6 Sublinear magnetisation

In a purely 2D system, Stoner approach yields the value of magnetisation \( M(H) \) which increases linearly with field from \( H = 0 \) all the way up to the saturation field \( H_s \). This is a consequence of the 2D density of states being energy-independent. When several 2D bands are present (corresponding in our case to different ladder and level indices \( l, a \)), the complete spin polarisation within a given band may be attained at field values \( H_{l,a}^{\downarrow} < H_s \), corresponding to \( E_{l,a}^{\downarrow} > 0 \) [cf. Eq. \( \text{(11)} \)]. In addition, new bands \( l', a' \) may become available as the corresponding energy for spin-up particles drops below the chemical potential \( E_{l',a'}^{\uparrow} < 0 \); we denote the corresponding fields \( H_{l',a'}^{\uparrow} \).

The value of dynamic susceptibility \( \chi(H) \equiv \partial M/\partial H \) then shows jumps at \( H_{l,a}^{\downarrow} \), while remaining constant elsewhere. These constant values of \( \chi(H) \) between the jumps depend on the thermodynamic formulation of the problem – whether it corresponds to the chemical potential (more precisely, \( \mu - E_{cs} \)) or net carrier density \( n \) being fixed. As mentioned in Sect. 2, our system is closer to the latter regime (see below).

The results of numerical calculation of \( M(H) \) for our system at three different \( H = 0 \) carrier densities in the metallic regime are shown in Fig. 10 (a). We see that \( M(H) \) increases monotonically and continuously all the way up to saturation; there is no evidence of a discontinuity at \( H = H_s \), which was reported in the case of a 2DEG with Coulomb repulsion. For higher densities, one observes pairs of features (cusps), merged together on the scale of the figure. For \( n = 3.14 \times 10^{13} \) cm\(^{-2} \), these correspond to \( H_{0,1}^{\downarrow}/H_s \approx 0.056 \) and \( H_{1,0}^{\downarrow}/H_s \approx 0.067 \), whereas for \( n = 6.62 \times 10^{13} \) cm\(^{-2} \) we find \( H_{0,1}^{\downarrow}/H_s \approx 0.062 \) and \( H_{1,0}^{\downarrow}/H_s \approx 0.079 \) (owing to a larger combined density of states \( \gamma_{l,n_{\downarrow}} \), \( H_{1,0}^{\downarrow} \) corresponds to a stronger feature). For \( n = 2.63 \times 10^{12} \) cm\(^{-2} \), there are two weak barely visible features corresponding to \( H_{1,0}^{\downarrow} \approx 0.20H_s \) and \( H_{1,0}^{\uparrow} \approx 0.42H_s \).

As explained in Sect. 2 our calculation is performed at a fixed value of the gate voltage \( \phi_{\text{gate}} \), thus modelling the actual experimental setup. We find that for the zero-field density \( n = 6.62 \times 10^{13} \) cm\(^{-2} \) increasing value of \( H \) from 0 to \( H_s \) leads to a decrease of the absolute value of \( E_{cs} \) by some 5\%, whereas the density \( n \) increases by about 0.003\%. Corresponding values for the other two curves on Fig. 10 are similar. We see that indeed the system is much closer to the fixed-\( n \) regime than to that of a constant \( E_{cs} \). We note that in all cases,
(a) Numerical results for the degree of spin polarisation in the paramagnetic phase, $2M/n$, plotted as a function of renormalised magnetic field $H/H_s(n)$, where $H_s(n)$ is the saturation field. Solid, dashed, and dotted line correspond, respectively, to the following $H = 0$ values of density $n$: $2.63 \cdot 10^{12}$ cm$^{-2}$ ($H_s \approx 25$ meV in energy units), $3.14 \cdot 10^{13}$ cm$^{-2}$ ($H_s \approx 139$ meV), and $6.62 \cdot 10^{13}$ cm$^{-2}$ ($H_s \approx 198$ meV). (b) The relative change of magnetic susceptibility $\chi$ at low fields for the same values of $n(H = 0)$.

the value of magnetic length

$$l_B = \left( \frac{\hbar c \mu_B}{eH} \right)^{1/2} = \frac{\hbar}{\sqrt{2m_e H}}$$

(41)

at $H = H_s$ is two to three times smaller than the average value of $z$ for the carriers, suggesting the importance of orbital effects of the in-plane field. While we do not take these effects into account, we note that elsewhere [21] these were found to result in a slight upward bend (superlinear behaviour) of the $M(H)$ curve at $U = 0$ at low densities.

It may appear that the behaviour of $M(H)$ as shown in Fig. 10 (a) is linear except for the features at $H_{1,0}^\uparrow$. In reality, this holds only for the lowest density, $n = 2.63 \cdot 10^{12}$ cm$^{-2}$, where the effects of short-range interaction are too weak to affect the transverse carrier motion. This is illustrated by Fig. 10 (b), depicting relative change of the dynamic susceptibility with $H$ at low fields. The pairs of susceptibility jumps at $H = H_{1,0}^\uparrow$ and $H = H_{1,0}^\downarrow$ are seen for higher densities. In addition, the appreciable decrease of $\chi(H)$ with $H$ at $H < H_{0,1}^\downarrow$ implies a sublinear magnetic field dependence of $M$ in this region. This behaviour becomes more pronounced as the density increases toward the ferromagnetic instability.

This sublinear behaviour of magnetisation is due to the effect of carrier wave functions changing with increasing $M$, as discussed above. Indeed, the effective interaction $U_{2D}$ enhances the magnetic susceptibility in comparison

\[\text{Note that our } H \text{ is defined in the units of Bohr magnetone.}\]

\[\text{At these low fields, our omitting the orbital effects is mathematically justified.}\]
to its non-interacting value. With increasing $M$, the wave-function profiles are adjusted in such a way that the interaction energy is lowered. Hence the effective value of $U_{2D}$ decreases (see Sect. 2) and so does the susceptibility.

The sublinear field dependence of $M$ is of crucial importance for one feature of the present theory which is not expected in the conventional Stoner treatment of a purely 2D system, viz., the continuous character of ferromagnetic transitions (Sects. 3, 4, 5). Indeed, a simple Landau–Ginzburg type description implies that a continuous transition requires the presence of a positive quartic (in $H$) term in the free energy, and hence sublinear magnetisation. It is hoped that perfecting the magnetisation measurement techniques and extending them to the higher-density region (where the long-range correlations become negligible) will allow to directly confirm this behaviour in a Si-MOSFET.

7 Conclusion

We constructed a mean-field description of electrons in an inversion layer, addressing both the behaviour of the system in the metallic high-density region and the correlated low-density regime immediately above the metal-insulator transition. Such electronic systems [as exemplified by Si-(100) MOSFETs] are characterised by the presence of both long-range Coulomb repulsion and the ubiquitous short-range (on-site, Hubbard) interaction. Coulomb interaction was treated at the mean-field level following Ref. [31], which leaves out long-range correlation effects, important in the low-density limit where the dimensionless parameter $r_s = m^*_e e^2/(\hbar^2 \sqrt{\pi n_1})$ is large (we included these effects phenomenologically in Sect. 4).

We recall that in a bulk three-dimensional system of electrons interacting via contact potential, Eq. (1), the strength of this interaction is measured by the dimensionless quantity $k_F a_{3D}$, where $k_F$ is the Fermi wave vector and $a_{3D} = m_e U/4\pi \hbar^2$ (where $m_e$ is the appropriate 3D effective mass) is the scattering length in the Born approximation. Therefore one expects that in a dilute system (small $k_F a_{3D}$, large $r_s$) the effects of short-range interaction are negligible. At larger densities, the increasing value of $k_F a_{3D}$ gives rise to stronger Fermi-liquid renormalisations (in particular, enhancing the magnetic susceptibility); at the same time, smaller values of $r_s (\propto m^*_e e^2/(\hbar^2 n_1^{1/3})$ in the three-dimensional case) and enhanced screening eventually permit neglecting the long-range Coulombic correlations. Depending on the properties of the system, it may or may not undergo a Stoner transition, accompanied by a susceptibility divergence.

In a restricted geometry of an inversion layer (a quasi-2D system), this picture is modified in a drastic way. Momentum dependence of the $s$-wave scattering amplitude in 2D (see, e.g., Ref. [45]) yields the momentum-dependent scattering length $a_{2D}(k)$. Assuming for simplicity that only one level of

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10 Here, the scattering length is defined using the reduced mass of a pair of identical particles, i.e., in this case, $m_e/2$. 

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transverse motion is active (electrical quantum limit, Sect. 3 above), one finds for a given 2D wave vector $k$, in the Born approximation for the contact interaction, Eq. (10):

$$\log \frac{2}{k a_{2D}} = \frac{2\pi h^2}{m_\perp U_{2D}} + \gamma_E.$$  \hspace{1cm} (42)

Here, $\gamma_E \approx 0.577$ is Euler’s constant. The (short-range) interaction strength parameter in the 2D case is given by $g = \left[ \log \left( \frac{2}{k_F a_{2D}} \right) \right]^{-1}$. According to Eq. (42), in the absence of long-range correlations the value of $g$ depends on the 2D density $n$ only via $U_{2D}$. While the latter does grow with $n$ owing to decreasing inversion layer thickness (the latter, as dictated by electrostatics), this growth is relatively slow (see Fig. 2). Indeed, we estimate that as the density varies from $8 \cdot 10^{10}$ cm$^{-2}$ to $8 \cdot 10^{13}$ cm$^{-2}$, the value of $g$ increases from about 0.03 to 0.12. This increase, implying an appreciable effect of interaction at larger densities, is expected to be more pronounced in a real multi-level system, where the valleys with larger in-plane mass are populated.

In a 2D system where there is no coexistence of broad and narrow partially-filled bands at the Fermi level, the short-range interaction is generally not expected to easily yield ferromagnetism (as exemplified by the square-lattice Hubbard model, see, e.g., Refs. [23,24,25]). Even in the range of densities where the ferromagnetism does occur, the required interaction strength is so large that Stoner mean-field approach is clearly irrelevant (see, however, Ref. [28]). However, in the case of a silicon inversion layer at high densities, there is an additional mechanism (transverse wave function dependence on magnetisation) acting alongside the conventional Stoner one (viz., the mean-field shifts of band energies). This opens an additional avenue toward ferromagnetic instability in the range where mean field approach is still expected to be applicable (see Appendix). In the opposite case of very low densities just above the MIT, the interaction-induced wave-function changes are negligible, yet there is a strong renormalisation of carrier properties due to the long-range Coulomb correlations [13,22,38,42]. In this case as well, we suggest that the Stoner approach is at least qualitatively relevant (see Appendix for details). While we do obtain a ferromagnetic instability at a density slightly above the critical value where the carrier effective mass diverges, a proper theoretical treatment, including both short- and long-range interactions from the beginning, is still missing.

We are now in a position to summarise our results in more detail, beginning with the low-density regime above the MIT, which is characterised by strong long-range correlations. In Sect. 4 these were taken into account phenomenologically via effective mass renormalisation, Eq. (30), as observed experimentally [22] and predicted theoretically [13]. While this mass renormalisation alone would lead to an increased magnetic susceptibility [22], we find

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11 Eq. (42) is obtained from the requirement [46] that scattering phase shifts for the contact and hard-core potentials coincide.

12 Which is expected to provide a valid estimate throughout our range of values of parameters, see Appendix.

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that including the effects of on-site repulsion enhances susceptibility further, leading to a second-order ferromagnetic transition. The latter takes place at a density which is a few per cent above the value corresponding to the (asymptotic) divergence of the effective mass. This difference is relevant in the context of the disagreement between presently available experimental results.\cite{59,11} Further experiments are needed in order to shed light on this controversy, and also to clarify whether the MIT corresponds to the effective mass divergence or (as we speculated) to the magnetic transition.

The origins of such a strong effect of short-range interactions at low densities become clear as we note [see Eq. (42)] that, for example, a five-fold increase in the effective mass $m_\perp$ has the same effect on the value of $k_F a_{2D}$ as does the five-fold increase of $U_{2D}$ (for example, at $n = 8 \cdot 10^{10}$ cm$^{-2}$, the value of $g$ would increase to 0.14; we verified that a self-consistent change of $U_{2D}$ due to the increase of $m_\perp$ is negligible, as expected). Specifically, the system even at $n \sim n_c$ becomes strongly interacting also in terms of short-range interaction. We also remark that a strong short range interaction can lead to strong renormalisation of the Fermi liquid parameters (including an additional renormalisation of the effective mass), which was not taken into account in our work or elsewhere. This highlights the need for a microscopic theory which would include both long- and short-range interactions on the same footing.

In the metallic regime at high densities, where the long-range correlation effects become unimportant, the value of $ka_{2D}$ increases due to the increasing $U_{2D}$ (see above). On the other hand, the wave functions begin to change under the effects of an applied field (see Fig. 3), as the mean field energy scale $nU_{2D}$ becomes sufficiently large to perturb the transverse carrier motion. These two effects lead to a strong increase in magnetic susceptibility $\chi$ with $n$, ultimately resulting in a ferromagnetic transition. For our parameter values, this takes place at $n_{FM} \approx 1.15 \cdot 10^{14}$ cm$^{-2}$, which is presently beyond the experimental range for a Si-MOSFET. However, this value was obtained (in Sect. 5) without taking into account the Fermi liquid renormalisations (such as effective mass enhancement, cf. Refs. \cite{47,48,49}), which again become important in this regime and may lower the value of critical density. Beyond mean-field description, fluctuation effects\cite{28} may lead to a further decrease of this quantity.

As explained above, the wave functions change under the effect of an applied field leads to relaxing the Stoner criterion of ferromagnetism. In terms of critical density, this means that the obtained value of $n_{FM}$ is lowered in comparison to naive Stoner-based estimates (which are invalid in the case of geometrically restricted systems such as inversion layer). In addition, this gives rise to a non-linear field dependence of magnetisation. The latter was discussed previously for the case of quasi-2D systems with Coulomb interaction\cite{21,43,44}, albeit at smaller densities, and our results outlined in Sect. 6 thus provide an additional mechanism for such non-linearity.

Whether the actual high-density ferromagnetic transition is reachable or not, the minimum and the subsequent increase of $\chi$ with density at $n \gtrsim 2 \cdot 10^{12}$ cm$^{-2}$ should be observable. We also note that the threshold density $n_0^{(0,1)} \approx$
3.3 \cdot 10^{12} \text{ cm}^{-2}$, beyond which the second transverse level is populated at $H = 0$, is not far from the highest value used in the measurements to date ($n = 2.08 \cdot 10^{12} \text{ cm}^{-2}$, see Ref. [5]), and should be attainable experimentally. In addition to new and potentially interesting transport phenomena arising at this point, one should be able to measure the associated jump in the susceptibility $\chi$ (cf Fig. 8). With the help of Eq. 38, this can be used to calibrate $U^{(2D)}$, and ultimately $U$. Note that the value of $n^{(0,1)}$ can be further reduced by decreasing the acceptor density $N_A$.

In order to keep our description simple, we omitted a number of effects which are expected to be of quantitative importance only. These include a more accurate formulation of the wave-function boundary conditions at $z = 0$ (Ref. [31]), the image-charge potential [2], etc. Significantly, we also disregard the effects of the valley degree of freedom, where an accurate description would involve using the appropriate values (not yet available) for the strength of short-range interaction between the carriers belonging to different valleys. Note that once such more accurate model is constructed, the important issue of valley “polarisation” [33] can be treated in the same way as that of spin polarisation.

In the present work, we specifically aimed at describing Si-(100) MOSFETs, however our results are expected to be qualitatively relevant for other 2D electron systems of finite thickness. These general conclusions are: (i) At higher densities, proper treatment requires taking into account the wave function change under the applied in-plane magnetic field [13] (see Fig. 3). This effect leads to an increased susceptibility in the paramagnetic state and enhances the tendency toward ferromagnetism. (ii) When the long-range correlations at low densities lead to the effective mass enhancement (as in Si-MOSFET [22] or in GaAs quantum wells [38]), magnetic properties are significantly affected by the on-site carrier repulsion, which can lead to a ferromagnetic instability.

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APPENDIX: On the applicability of Stoner-type mean field approach in low-density 2D systems

In this work, we consider low-density (quasi-)2D electrons, and one might ask whether the short-range repulsion can affect the properties of the system in our range of values of parameters. If the answer were in the negative, this would have turned our mean-field treatment into an artifact of an inadequate
approach. It is therefore important to consider this issue in more detail (in addition to discussing the scattering length in Sect. 7).

For simplicity, we consider a purely 2D system,

\[ H = \sum_i \frac{p_i^2}{2m_\perp} + \frac{1}{2} \sum_{i \neq j} U_{2D}(\mathbf{r}_i - \mathbf{r}_j), \]

(A.1)

where the summations are over the particle numbers. The effective 2D interaction \( U_{2D} \) is in our case given by Eq. (10); calculations of Sect. 3 (cf. Fig. 2) yield the value of \( U_{2D} \approx 1.2 \cdot 10^{-27} \text{erg}\cdot\text{cm}^2 \) at \( n = 8 \cdot 10^{10} \text{cm}^{-2} \) and \( U_{2D} \approx 5.3 \cdot 10^{-27} \text{erg}\cdot\text{cm}^2 \) at \( n = 8 \cdot 10^{13} \text{cm}^{-2} \). The level indices are suppressed as presently we are considering the single-level case. Now let us consider interaction of a sole spin-down electron with the spin-up Fermi sea. The mean-field result for the net interaction energy is of course \( \delta E_{\text{mf}} = U_{2D} n_\uparrow \) (where at \( M = 0, n_\uparrow = n/2 \)), and our worry is that this expression may be a gross overestimate. Indeed, with increasing \( U_{2D} \) spin-up electrons will be avoiding the site occupied by the spin-down electron, resulting in a smaller energy change which retains a finite value \( \delta E_\infty \) (of the order of the Fermi energy or less) even as \( U_{2D} \) increases to infinity. The situation may arise where actually

\[ \delta E_\infty < \delta E_{\text{mf}} = U_{2D} n/2, \]

(A.2)

in which case we suspect that the mean field estimates become irrelevant. Note that in reality there is a finite concentration of spin-down particles and the perturbations of spin-up Fermi sea by individual spin-down electrons are not independent, so that \( n_i \delta E_\infty \) underestimates the interaction energy at large \( U_{2D} \). In order to estimate \( \delta E_\infty \), we first evaluate the energy change \( \Delta E \) of a spinless two-valley ideal 2D Fermi gas \( (H_0 = p^2/2m_\perp) \) under the perturbing effect of a static impurity at origin [corresponding to potential energy \( V = V\delta(r) \)]. Using the Lifshitz–Krein trace formula[52], this is conveniently expressed as an integral from the bottom of the band to the Fermi energy,

\[ \Delta E(V) = 2 \int_{\epsilon_F}^{\epsilon_F^+} \xi(\epsilon) d\epsilon. \]

(A.3)

Here, the prefactor corresponds to the two independent valleys, and the spectral shift function \( \xi \) [with the property that \(-d\xi/d\epsilon\) equals \( \delta \nu(\epsilon) \), an impurity-induced correction to the density of states \( \nu(\epsilon) \)] is given by[52,53,54]

\[
\xi(\epsilon) = -\frac{1}{\pi} \text{Arg Det} \left\{ 1 - \frac{1}{\epsilon - i0 - H_0} V \right\} = \\
= -\frac{1}{\pi} \text{Arg} \left\{ 1 - V \int \frac{d^2k}{4\pi^2} \frac{1}{\epsilon - i0 - (k^2/2m_\perp)} \right\} = \\
= -\frac{1}{\pi} \text{Arg} \left\{ 1 - V \int_{\epsilon'}^W \frac{\nu(\epsilon') d\epsilon'}{\epsilon - \epsilon'} - \pi i \nu(\epsilon) \right\}. \quad \text{(A.4)}
\]

Here, the momentum integral is over the Brillouin zone, whereas the energy integral in the last line is over the entire band, \( 0 < \epsilon' < W \).
Since we will ultimately need to integrate $\xi$, the weak singularity at $\epsilon = 0$ is unimportant. In the low-density case of $\epsilon_F \ll W$ we estimate
\[
\int_0^W \nu' \frac{d\epsilon'}{\epsilon - \epsilon'} \sim \nu_0 \log \left( \frac{\epsilon}{W} \right) \sim \nu_0 \log \left( \frac{\epsilon_F}{W} \right) \sim \nu_0 \log \left( \frac{n_\uparrow}{2N_0} \right),
\]
with $\nu_0$ given by Eq. (12), and $N_0 \sim 1/a^2$ (where $a$ is the lattice period), the full capacity of the 2D band for fixed spin and valley indices. Thus, we find
\[
\xi(\epsilon) \approx \frac{1}{\pi} \arctan \frac{\pi V \nu_0}{1 - V \nu_0 \log(n_\uparrow a^2/2)}. \tag{A.5}
\]
Spectral shift function is related\textsuperscript{14} by the Friedel sum rule to the scattering phase shift\textsuperscript{[56]}, with the Born approximation corresponding to omitting the logarithmic term in Eq. (A.5). At small $V$, Eq. (A.3) then yields the expected perturbative result $\Delta E = V n_\uparrow$, whereas for large $V \gtrsim 1/|\nu_0 \log(n_\uparrow a^2/2)|$ we find
\[
\Delta E(\infty) \approx 2\epsilon_F \left| \log(n_\uparrow a^2/2) \right|^{-1}. \tag{A.6}
\]
The latter is the energy change of spin-up Fermi sea when a node at $r = 0$ is created in all the electron wave functions. It is seen that indeed at very low densities $\Delta E(\infty)/\epsilon_F$ vanishes logarithmically, which is the physical reason why the short-range interaction becomes irrelevant at sufficiently low densities. In our case, however, the absolute value of the log does not exceed 10.

In addition, note that the quantity $\delta E_\infty$ involves interaction with a spin-down electron which is not localised at origin but is moving with a velocity of order of $v_F$. The wave-functions node is presumably a heavy object, and moving it along would result in a large addition to $\Delta E(\infty)$. It is thus more economical to have the spin-down electron localised in an area of size $R \sim \hbar/p_F$ (which can be done without appreciably changing its energy) while requiring that the wavefunctions of the spin-up electrons vanish throughout this area. The corresponding energy change of the spin-up Fermi sea is a sum of $\Delta E(\infty)$ and an area term, needed to “inflate” the node to the required finite area:
\[
\delta E_\infty \sim \Delta E(\infty) + 2\epsilon_F \int_0^{\epsilon_F} \epsilon d\epsilon R^2 = 2\epsilon_F \left| \log(n_\uparrow a^2/2) \right|^{-1} + \frac{1}{4\pi} \epsilon_F. \tag{A.7}
\]
Throughout our range of parameter values, the second term is at least several times smaller than the first one, hence we do not need a more elaborate estimate of the energy of correlated motion of spin-down electron. We are now in a position to quantitatively verify that we never approach the “dangerous” regime specified by the inequality (A.2). Since presently we did not take into account the possibility of multiple occupied subbands (which is not expected to qualitatively affect the results), this must be done with the help of the numerical results obtained for the single-level case, Sect. 3.

\textsuperscript{14} For a recent mathematical discussion, see Ref. [55].
Using the values of $U_{2D}$ quoted above, we find that at $n = 8 \cdot 10^{10}$ cm$^{-2}$ (where the Fermi energy as measured form the bottom of the band is $\epsilon_F \equiv E_v - E_0 \approx 0.51$ meV), the value of $\delta E_{mf} \approx 0.029$ meV is about 5 times smaller than $\delta E_{\infty} \approx 0.15$ meV. Likewise, at $n = 8 \cdot 10^{13}$ cm$^{-2}$ (where $\epsilon_F \approx 0.51$ eV), the value of $\delta E_{mf} \approx 132$ meV is smaller than $\delta E_{\infty} \approx 400$ meV.

We thus conclude that the mean-field estimate of the interaction energy, and by extension the Stoner approach, should be at least qualitatively applicable throughout the entire range of densities considered herein. Since a Stoner-type treatment is anyhow not expected to be quantitatively accurate, this is a satisfactory outcome.

One further note should be made concerning the situation at very low densities near MIT (Sect. 4). In this case, the long-range forces lead to a significant reduction of effective band width (and hence of the effective Fermi energy), to the extent that if those renormalised quantities are substituted when calculating $\delta E_{\infty}$, one might find that the inequality (A.2) is actually satisfied. We wish to argue that such a substitution would be hard to justify, quoting the following reasons:

(i) the renormalised quantities refer not to the electrons, but to the resultant quasiparticles. These are extended objects, which presumably should be viewed as residing on an effective lattice with proportionally increased lattice period, which should thus be used in place of $a$ in Eq. (A.7).

(ii) More importantly, these quasiparticles characterise low-energy, long-wavelength properties of the system, whereas contact interaction with point defects involves a significant short-wavelength component. The short-wavelength contribution to Eq. (A.3) originates from the logarithmic term in Eq. (A.5). Therefore, it is more appropriate to use unrenormalised spectral parameters when estimating this term only, including the coefficient before the logarithm. Elsewhere in Eqs. (A.3) and (A.5), one should be using the renormalised spectrum characterised by a larger mass, yet it is easy to see that within this order-of-magnitude estimate the renormalisation coefficient cancels out for large $V$. Hence $\delta E(\infty)$ retains (roughly) its unrenormalised value and we arrive at a conclusion that the mean-field approach is still qualitatively applicable.

References

1. A. B. Fowler, F. F. Fang, W. E. Howard, and P. J. Stiles, Phys. Rev. Lett. 16, 901 (1966).
2. T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. 54, 437 (1982).
3. S. V. Kravchenko, G. V. Kravchenko, J. E. Furneaux, V. M. Pudalov, and M. D’Iorio, Phys. Rev. B50, 8039 (1994).
4. S. V. Kravchenko and M. P. Sarachik, Rep. Prog. Phys. 67, 1 (2004), and references therein.
5. B. Spivak B., S. V. Kravchenko, S. A. Kivelson, and X. P. A. Gao, Rev. Mod. Phys. 82, 1743 (2010), and references therein.
6. I. Shlimak, A. Butenko, D. I. Golosov, K.-J. Friedland, and S. V. Kravchenko, Europhys. Lett. 97, 37002 (2012).
7. D. I. Golosov, I. Shlimak, A. Butenko, K.-J. Friedland, and S. V. Kravchenko, Phys. Rev. B88, 155313 (2013).
8. S. V. Kravchenko, A. A. Shashkin, S. Anissimova, A. Venkatesan, M. R. Sakr, V. T. Dolgopolov, and T. M. Klapwijk, Ann. Phys. 321, 1588 (2006).
9. A. A. Shashkin, S. Anissimova, M. R. Sakr, S. V. Kravchenko, V. T. Dolgopolov, and T. M. Klapwijk, Phys. Rev. Lett. 96, 036403 (2006).
10. V. M. Pudalov, A. Yu. Kuntsevich, I. S. Burmistrov, and M. Reznikov, J. Low Temp. Phys. 181, 99 (2015), and references therein.
11. O. Prus, Y. Yaish, M. Reznikov, U. Sivan, and V. Pudalov, Phys. Rev. B67, 205407 (2003).
12. N. Teneh, A. Yu. Kuntsevich, V. M. Pudalov, and M. Reznikov, Phys. Rev. Lett. 109, 226405 (2012).
13. A. Punnoose and A. M. Finkelstein, Science 310, 289 (2005).
14. B. Tanatar and D. M. Ceperley, Phys. Rev. B39, 5005 (1989).
15. C. Attaccalite, S. Moroni, F. Gori-Giorgi, and G. B. Bachelet, Phys. Rev. B67, 205407 (2003).
16. N. Teneh, A. Yu. Kuntsevich, V. M. Pudalov, and M. Reznikov, Phys. Rev. Lett. 109, 226405 (2012).
17. A. A. Shashkin, S. V. Kravchenko, V. T. Dolgopolov, and T. M. Klapwijk, Phys. Rev. Lett. 87, 086801 (2001).
18. S. A. Vitkalov, H. Zheng, K. M. Mertes, M. P. Sarachik, and T. M. Klapwijk, Phys. Rev. Lett. 87, 086401 (2001).
19. A. A. Shashkin, S. V. Kravchenko, V. T. Dolgopolov, and T. M. Klapwijk, Phys. Rev. B66, 075303 (2002).
20. V. T. Dolgopolov, JETP Lett. 101, 282 (2015) [Zh. Eksp. Teor. Fiz. Pis’ma Red. 101, 300 (2015)].
47. J. R. Engelbrecht and M. Randeria, Phys. Rev. B 45, 12419 (1992).
48. J. R. Engelbrecht, M. Randeria, and L. Zhang, Phys. Rev. B 45, 10135 (1992).
49. P. Bloom, Phys. Rev. B 12, 125 (1972).
50. I. L. Kurland, I. L. Aleiner, and B. L. Altshuler, Phys. Rev. B 62, 14886 (2000).
51. A. U. Sharafutdinov, D. S. Lyubshin, I. S. Burnistrov, Phys. Rev. B 90, 195308 (2014).
52. I. M. Lifshits, Usp. Mat. Nauk 7, No. 1, 171 (1952) (in Russian).
53. I. M. Lifshits, S. A. Gredekul, and L. A. Pastur, Introduction to the Theory of Disordered Systems (J. Wiley & Sons, New York, 1988), Chapt. 5.
54. M. G. Krein, Topics in Differential Equations and Operator Theory (Birkhäuser, Basel, 1983), pp. 107-172.
55. M. Kohmoto, T. Koma, and S. Nakamura, Ann. Henri Poincaré 14, 1413 (2013).
56. I. M. Lifshits, Uchenye Zapiski Kharkovskogo Gos. Universiteta 27, 105 (1948) (in Russian).