Many-Body Effects in Spin-Polarized Two-Dimensional Electron Gas

Jumpei Terada and Tsuneya Ando
Department of Physics, Tokyo Institute of Technology
2-12-1 Ookayama, Meguro-ku, Tokyo, 152-8551, Japan.

Abstract

Many-body effects on the spin polarization are studied in an n channel inversion layer on Si (100) surface in a magnetic field parallel to the surface in random phase approximation. The spin polarization exhibits a discrete jump to a full polarization at the critical magnetic field in the low-density regime and the critical field is reduced considerably from that estimated by an extrapolation based on the zero-field susceptibility.

Key words: Many body effects, Spin polarization, Parallel magnetic field, Ferromagnetic instability
PACS: 72.10-d, 73.20-r, 73.23-b

The importance of interaction in two-dimensional electron systems has been well-established as a result of extensive study [1]. In fact, measurements and calculations of quasi-particle properties such as the effective mass and the effective g-factor were performed [1]. A transition between paramagnetic and ferromagnetic ground states was studied also [2,3]. Further, a complete spin polarization was realized at low electron concentrations in a strong parallel magnetic field [4–12].

In this study, the spin polarization of a Si n channel inversion layer in a parallel magnetic field is calculated in various approximations such as the Hartree approximation (HA), the Hartree-Fock approximation (HFA), and the random-phase approximation (RPA).

In an n channel inversion layer on the Si (100) surface, there are two valleys with a heavier mass $m_l/m_0 = 0.916$ in the direction perpendicular to the surface and four valleys with a lighter mass $m_t/m_0 = 0.1905$. The lowest subband is composed of the former two valleys and therefore we shall confine ourselves to the corresponding subband. Effects of a parallel magnetic field are included only as the spin Zeeman energy and those on the subband wave function in the z direction perpendicular to the surface are completely neglected. This is a reasonably good approximation in the inversion layer because of the strong confinement in the z direction.

We use the variational function

$$\zeta_\sigma(z) = \sqrt{b_\sigma^2/2} \exp \left( -\frac{b_\sigma^2}{2} z^2 \right),$$

with variational parameter $b_\sigma$ [13]. This variational function gives the average $\langle z \rangle_\sigma = 3/b_\sigma$. In the presence of spin polarization, $b_\sigma$ depends on spin $\sigma$ (+ for up spin and — for down spin).

Apart from the spin Zeeman energy, the Hartree part of the total energy per an electron is given by

$Preprint submitted to Physica E 1 July 2005$
\[
\frac{E_{\text{Hartree}}}{N} = \sum_{\sigma=\pm} \left[ \frac{\pi N_s \hbar^2}{m_i g_e} \frac{1}{4} (1 + \sigma \Delta)^2 + \frac{1 + \sigma \Delta}{2} \left( \frac{\hbar^2 b_0^2}{8m_i} + \frac{12 \pi e^2 N_d}{\kappa_{\text{sc}} b_0} \right) \right] + \frac{\kappa_{\text{sc}} - \kappa_{\text{ins}}}{\kappa_{\text{sc}} + \kappa_{\text{ins}}} \frac{e^2 b_0}{8m_i} (3 + \frac{33 \pi^2 e^2 N_s}{8\kappa_{\text{sc}} b_0}),
\]

where \( N_s \) is the electron concentration per unit area, the valley degeneracy is given by \( g_e = 2 \), the static dielectric constant is \( \kappa_{\text{sc}} = 11.8 \) for silicon and \( \kappa_{\text{ins}} = 3.8 \) for SiO\(_2\), \( N_d \) is the charge density in the depletion layer, and \( \Delta \) is the spin polarization defined such that \((1+\Delta)N_s/2\) and \((1-\Delta)N_s/2\) are the density of up- and down-spin electrons, respectively. In the above equation, the first term represents the kinetic energy for the motion parallel to the surface and the second term the kinetic and potential energy for the perpendicular motion.

The exchange energy is given by

\[
E_{\text{corr}} = -\frac{N_s}{g_e} \sum_{\sigma} \left( \frac{1 + \sigma \Delta}{2} \right)^{3/2} \int_0^\infty dx k_F^2 x V_{\sigma\sigma}(k_F^2 x) \times \left( \cos \frac{\pi}{2} - \frac{\pi}{4} \sqrt{1 - x^2} \right),
\]

where the effective Coulomb interaction between an electron with spin \( \sigma \) and with spin \( \sigma' \) is given by

\[
V_{\sigma\sigma'}(q) = \frac{2\pi e^2}{\kappa_{\text{sc}} q} \int dz \int dz' \left( \frac{\epsilon q |z-z'|}{\kappa_{\text{sc}} \kappa_{\text{ins}}} - \frac{\kappa_{\text{ins}} q |z+z'|}{\kappa_{\text{sc}} q} \right)^2 \times \left( e^{-q |z-z'|} + \frac{\kappa_{\text{sc}} - \kappa_{\text{ins}}}{\kappa_{\text{sc}} + \kappa_{\text{ins}}} e^{q |z-z'|} \right),
\]

and \( k_F \) is the Fermi wave number of electrons with spin \( \sigma \). The correlation energy in RPA is given by [14]

\[
\frac{E_{\text{corr}}}{N} = \frac{1}{N_s} \int_0^\infty dq \int_0^{\infty} \frac{d\omega}{2\pi} \times \left\{ \ln(\det[1 + V(q)\Pi(q, \omega)]) - \text{Tr}V(q)\Pi(q, \omega) \right\},
\]

where \( V(q) \) and \( \Pi(q, \omega) \) are 2 \( 2 \) matrices in the spin space, given by

\[
V(q) = \begin{pmatrix} V_{++}(q) & V_{+-}(q) \\ V_{-+}(q) & V_{--}(q) \end{pmatrix},
\]

and

\[
\Pi(q, \omega) = \begin{pmatrix} \Pi_+ (q, \omega) & 0 \\ 0 & \Pi_- (q, \omega) \end{pmatrix},
\]

The polarization function is given by

\[
\Pi_\sigma(q, \omega) = g_e \int \frac{d\mathbf{k}}{(2\pi)^2} \frac{\theta(k_F^2 - k)}{\pi} \frac{\theta(k_F^2 - |\mathbf{k} + \mathbf{q}|)}{\omega + \epsilon_p - \epsilon_{p+q}},
\]

where \( \epsilon_k = \hbar^2 k^2/2m_i \). The integration over \( \mathbf{k} \) can be performed analytically.

In the following numerical calculation, the variational parameters \( b_0 \) and the spin polarization \( \Delta \) are determined by minimizing the total energy for a given set of \( N_s \), \( N_d \), and magnetic field \( B \) [14]. The critical magnetic field where electrons are fully polarized is denoted by \( B_c \). In the Hartree approximation, we have \( g_B B_c = 2E_F \), where \( g \) is the g factor (\( \approx 2 \)), the Bohr magneton is given by \( \mu_B = e\hbar/2m_i \), and \( E_F \) is the Fermi energy in the absence of spin polarization given by \( N_s = g_e m E_F / \pi \hbar^2 \). In the following we shall show results for \( N_d = 1 \times 10^{11} \text{ cm}^{-2} \), corresponding to a typical inversion layer with high quality.

Figure 1 shows an example of the total energy ob-
Fig. 2. The spin polarization as a function of the spin Zeeman energy. The solid straight line denoted by HA is the result in the Hartree approximation. The dotted straight line shows the result obtained by using the zero-field susceptibility, giving the critical field denoted by $B'_c$. The dotted curve denoted by $d\varepsilon/d\Delta$ is the polarization at a local minimum. The actual spin polarization exhibits a jump.

Fig. 3. The amount of the discrete jump of the polarization at the critical field as a function of the electron concentration (left vertical axis). The right vertical axis shows the spin Zeeman energy corresponding to a given spin polarization. The amount of the jump starts to appear around $N_s = 6 \times 10^{11}$ cm$^{-2}$, continuously increases with the decrease of $N_s$, and reaches unity around $N_s = 4 \times 10^{10}$ cm$^{-2}$, corresponding to the change of the ground state from paramagnetic to ferromagnetic. This critical density is in good agreement with the previous result for a similar value of $N_d$ [2].

Figure 4 compares the field of the complete polarization with that obtained by an extrapolation based on the zero-field susceptibility in RPA. The spin Zeeman energy for $N_s = 1 \times 10^{11}$ cm$^{-2}$.

First, we notice that the zero-field susceptibility is strongly enhanced and the critical field $B'_c$ obtained by extrapolation using the susceptibility is reduced considerably from the Hartree result. The actual critical field is further reduced and the reduction becomes larger with the increase of the polarization. A discrete jump to the perfect polarization occurs at $B_c$. As a result $B_c$ is less than a half of $B'_c$.

Figure 3 shows the amount of the jump at $B_c$ as a function of the electron density together with the spin Zeeman energy for a given spin polarization. The amount of the jump starts to appear around $N_s = 6 \times 10^{11}$ cm$^{-2}$, continuously increases with the decrease of $N_s$, and reaches unity around $N_s = 4 \times 10^{10}$ cm$^{-2}$, corresponding to the change of the ground state from paramagnetic to ferromagnetic. This critical density is in good agreement with the previous result for a similar value of $N_d$ [2].

Figure 4 compares the field of the complete polarization with that obtained by an extrapolation based on the zero-field susceptibility in RPA. The zero-field extrapolation works reasonably well and the deviation is less than 10% at a high electron density ($N_s > 2 \times 10^{12}$ cm$^{-2}$), but the deviation becomes appreciable at low electron concentrations ($N_s < 5 \times 10^{11}$ cm$^{-2}$).

Figure 5 compares the critical fields obtained in the Hartree approximation, Hartree-Fock approximation, and random phase approximation. In the Hartree approximation there is no discontinuous jump in the polarization. The Hartree-Fock results exhibit behavior
Fig. 5. The critical magnetic field $B_c$ calculated in the Hartree (HA), Hartree-Fock (HFA), and random phase approximation (RPA) as a function of electron density $N_s$. A dotted line shows that a discrete jump of the spin polarization occurs at the critical field.

qualitatively same as that of RPA results although different quantitatively. In fact, they show that a discontinuous ferromagnetic transition should occur around $N_s = 1 \times 10^{12} \text{cm}^{-2}$, which is more than one order of magnitude larger than the RPA prediction.

At low electron concentrations, the resistivity increases with the applied parallel magnetic field and reaches a plateau beyond a certain field [4,5]. The critical field for the complete spin polarization was estimated experimentally as the field where the resistivity reaches the plateau value [6,7,10] and was shown to be in reasonable agreement with that obtained theoretically from the zero-field extrapolation in RPA.

Although an exact comparison is not possible because the value of $N_d$ is not known well in experiments, the critical field obtained in the present work corresponds well to the field where the resistivity exhibits a steepest dependence on the field. It is more appropriate to identify the critical field in this way because of the presence of a band-tail due to disorder and nonzero temperature, and therefore the present result is in good agreement with the experiments. However, it is necessary to understand the origin of the strong dependence of the resistivity on the parallel magnetic field [8,9,11] and effects of a band-tail on the critical field for the exact identification of the critical field of the complete spin polarization.

Acknowledgments

This work has been supported in part by a 21st Century COE Program at Tokyo Tech “Nanometer-Scale Quantum Physics” from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

References


4