Ground State of a Quasi-Two-Dimensional Electron Gas

Yasumitsu Ito¹, Kazuyuki Okazaki² and Yoshihiro Teraoka¹

¹Department of Materials Science, College of Integrated Arts and Sciences, Osaka Prefecture University, Sakai 599-8531, Japan ²Interface Science Research Group, Special Division of Green Life Technology, AIST Kansai, Ikeda 563-8577, Japan

The ground state of an interacting electron gas is one of the most interesting problems from a fundamental point of view. A three-dimensional electron gas (3DEG) is expected to be a spin-unpolarized (NM) fluid in the high-electron-density limit and a spin-fully-polarized ferromagnetic (FPF) Wigner crystal at the low-density limit. Recently a novel concept was proposed for intermediate densities using the local spin density approximation (LSDA) [1-3]: electron-self-confined (ESC) state. The ESC state is interpreted in the LSDA as follows; electrons are self-confined to the valleys of an effective potential, which is periodic, induced by the electrons. There are three kinds of ESC state; Wigner film, Wigner rod and Wigner crystal (see Fig. 1). With decreasing electron density, the ground state of a 3DEG reveals three phase transitions from an NM fluid to an FPF Wigner film, to an FPF Wigner rod and finally to an FPF Wigner crystal. In treating an interacting electron gas, the positive-charge-background neutralizing an electron gas is described by a uniform jellium model. In a quasi-two-dimensional electron gas (Q-2DEG), it is a thin film with film thickness D.

In the present work, a magnetic phase transition in a Q-2DEG from an NM state to a magnetic state is investigated using the LSDA with Perdew-Zunger type exchange-correlation energy. The electronic and magnetic structures are calculated as a function of Wigner radius r_s and D. Figure 2 shows the magnetic phase diagram as a function of r_s and D. With increasing r_s for a given D, the ground state reveals a phase transition from an NM fluid to an FPF Wigner film via a spin-regionally-polarized ferromagnetic (RPF) state or a direct phase transition to an FPF state. An RPF state shows surface magnetism, which means that the spin polarization localizes only in the surface region. With increasing D, the phase boundary between NM fluid and FPF Wigner film approaches $r_s = 28.4$, at which a magnetic transition between NM fluid and FPF Wigner film occurs in a 3DEG. In the small limit of D, the ground state is FPF, not depending on r_s . However, a Q-2DEG with very small $D \leq r_s$ reveals another ground state; pencil-case structure in which Wigner rods are periodically arrayed (see Fig. 3) [4]. The contour map of the electron density profile in a section of a thin film is shown in Fig. 4, where D = 10and $r_s = 30$. The pencil-case structure appears at $D \lesssim 30$ for $r_s = 30$. The condition for an appearance of a pencil-case structure is given by $\sqrt{4r_s^3/(3D)} \lesssim 36$. On the other hand, Wigner ribbon appears in a 2DEG, instead of Wigner rod. However, there is an essential difference in physics between a 2DEG and a Q-2DEG with infinitesimal D; the ground state is NM in a 2DEG and FPF in a Q-2DEG with infinitesimal D. This originates from the fact that, in a 2DEG, the electron distribution is confined in a two-dimensional plane, on the other hand, electrons distribute outside the film in a Q-2DEG.

- [1] K. Okazaki and Y. Teraoka, Surf. Sci. 458, 15 (2000).
- [2] K. Okazaki and Y. Teraoka, Solid State Commun. **114**, 215 (2000).
- [3] K. Okazaki and Y. Teraoka, Appl. Surf. Sci. 169-170, 48 (2001).
- [4] K. Okazaki and Y. Teraoka, Solid State Commun. **116**, 269 (2000).



Figure 1: Schematic electron distributions in electron-self-confined (ESC) states, (a) Wigner film, (b) Wigner rod, and (c) Wigner crystal.



Figure 2: Magnetic phase diagram as a function of r_s and D in a Q-2DEG.



Figure 3: Schematic electron distributions of pencil-case structure in Q-2DEG.



Figure 4: The contour map of the electron density profile at D = 10 and $r_s = 30$.