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TRANSITIONS INTO NEW ORDERED STATES IN 2D ELECTRON FLUIDS

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The ground state energy of a quasi two-dimensional electron fluid is continuous for all densities but changes its analytical character at $r_s = \sqrt{2}$. The system falls into a liquid-like state at $r_s = 1.989$, where the compressibility diverges. Furthermore, electron correlations will induce a valley occupancy phase transition at $r_s = 8.011$. A similar mechanism will cause a spin polarized state at $r_s = 13.0$.

1. Introduction

Since Wigner's prediction, the crystallization of an electron gas has attracted considerable theoretical attention. The subject has become even more attractive recently because two-dimensional electron systems have been realized on the surface of liquid helium or at semiconductor interfaces. Different from the case of metals, the density of these electrons can be varied much widely so that experimental tests of Wigner's prediction have become conceivable. In fact, Grimes and Adams [1] have reported the first experimental evidence of a Wigner lattice for electrons on the surface of liquid helium. They have found that a phase transition from a liquid to a lattice takes place at electron density in the range $3\text{-}9\times10^8$ cm^{-2} and temperature between 0.35 and 0.65 ^{o}K. In terms of the familiar dimensionless parameter $\Gamma = e^2\sqrt{(\pi n)}/kT$, the transition occurs at 135 ± 15. Moreover, dislocation theory of two-dimensional melting has been applied successfully by Kosterlitz and Thouless and others [2].

These interesting works are all concerned with classical electrons. On the other hand, the electrons in inversion or accumulation layers of Si MOSFETs and at the interface of GaAs/GaAlAs superlattices can have higher densities and be quantum mechanically degenerate. They interact with each other through Coulomb forces so that they form quasi two-dimensional systems. To these electrons, the Kosterlitz and Thouless theory is not applicable. Furthermore, it is designed for describing melting rather than crystallization.

For degenerate electrons near absolute zero, the ground state energy plays a role of prime importance. Unfortunately, many electron theory has been developed in the past in the high density limit. Since interesting phase transitions are expected in intermediate/low density regions, efforts have been made to extend the high density approach. For instance, Isihara and Montroll [3] used Padé approximants to interpolate the high density gas energy and a low density lattice energy.

There is a fundamental reason why a high density approach has been developed. At high densities, the electrons are in a gaseous state so that Coulomb effects can be treated by perturbation. Such a treatment has been adopted by Isihara and Toyoda [4] in a way similar to Gell-Mann and

Brueckner's for three dimensions [5]. Unfortunately, the high density approach is restricted to very small r_s.

A breakthrough in many electron theory has been achieved by Isihara and Ioriatti [6]. They have found taht the eigenvalues of the electron propagator have an interesting electrostatic analogue: They represent the electric flux emerging from a conducting disc with a uniform charge distribution. Based on this analogue, they have discovered a natural coordinate system which suits the geometry of the flux and simplifies the eigenvalue expression. Since the correlation energy is determined by the eigenvalues, they have obtained an exact but very simple finite integral for the energy. This integral is similar to Onsager's energy integral for an Ising lattice except that it is more complicated and is characterized by r_s instead of Onsager's J/2kT.

In view of the development, we shall discuss in the present work some interesting transitions into new phases in quasi two-dimensional electron systems near absolute zero. We shall use the familiar r_s parameter which is defined by $r_s = 1/\sqrt{(\pi n)}$ where n is the electron density. We shall discuss what would happen when r_s is increased from zero.

2. Transition into a Liquid State

In the high density limit where r_s is very small, the ground state energy is dominated by the kinetic energy which is positive, and the system is gaseous. As r_s increases, the ground state energy drops very rapidly to zero around r_s= 0.7 and then becomes negative. Beyond this point, the electrons will be more and more correlated so that some changes in their properties are expected. However, the ground state energy is smooth and does not show a singularity.

Nevertheless, at $r_s = \sqrt{2}$ the analytical form of the ground state energy changes. Beyond this point, one can no longer use the high density series such as obtained by Isihara and Toyoda. In fact, we have derived a new low density series which is characterized by non-integral powers such as $r_s^{-4/3}$ or $r_s^{-2/3}$. Shortly beyond this dividing point, the energy reaches its minimum of -0.46 Ryd at $r_s = 1.475$. According to the Padé approximants of Isihara and Montroll, the three-dimensional minimum -0.163 Ryd appears at $r_s = 3.77$. Hence, comparing these two sets of figures, we can conclude that electron correlations are much stronger in two dimensions.

Because the energy is continuous and motivated by the dislocation theory, we have evaluated the isothermal compressibility. The result is illustrated in Fig. 1 as a function of r_s. The compressibility stays very small until around $r_s = 1$ where it starts increasing very rapidly. Finally, it diverges at $r_s^c = 1.989$. This divergence is approximately expressed by

$$\kappa \sim \frac{1}{|r_s - r_s^c|}$$

Note that both the energy minimum and this divergence occur at rather small r_s.

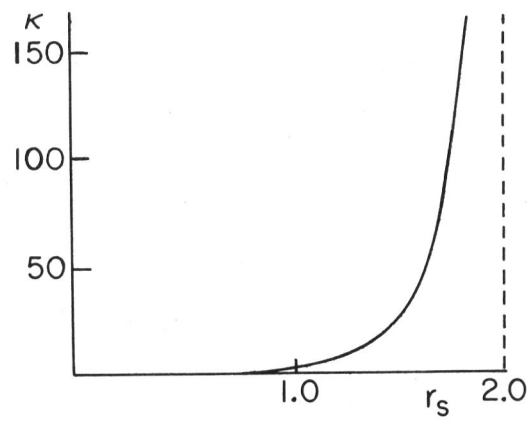

Fig. 1 Isothermal compressibility in (Bohr rad.)^2/Ryd as a function of r_s.

3. Valley Occupancy Transition

The conduction band of silicon consists of ellipsoidal constant-energy surfaces in six crystal directions. In silicon inversion layers, motion of electrons perpendicular to the surface is restricted under a confining potential so that the energy is quantized into a series of subbands. This multi-valley status of the band gives rise to a valley degeneracy factor ν. In the [100] direction, two equivalent valleys have their major axes with a high effective mass perpendicular to the surface, while the other four have their major axes and a lower normal effective mass in the plane of the surface. Consequently, the ground subband is expected to have a valley degeneracy $\nu = 2$.

Although the two valleys should in principle be occupied by the electrons equally, Bloss, Sham and Vinter [7] have suggested that electron correlations may lift the symmetry. More recently, Cole and others [8] have performed spectroscopic measurements of transition energies between the [100] subbands of Si and reported a pronounced sudden change in the slope of the transition energies at electron density 5×10^{11} cm^{-2}. They have attributed this change to a valley occupancy transition from a two-valley state to a one-valley state.

The valley transition should be a low density phenomenon. We remark that the Fermi energy is given for arbitrary ν by $p_o^2 = 2\pi n/\nu$. Hence, a one-valley state has a higher Fermi energy than a two-valley state. Accordingly, its kinetic energy is also higher. Unless the density is reduced considerably, a one-valley state is not favorable energetically.

At low densities, the ground state energy is small. Also, the ground state energies for the two states decrease similarly to each other. Therefore, it has been rather difficult to determine accurately their crossing point which should be the transition point.

Our all density theory can be effectively employed in this respect. We have found that the energy difference $\Delta\varepsilon$ between the one-valley and two-valley states is given by

$$\frac{\Delta\varepsilon}{\varepsilon_o} = 1 - 0.14\, r_s^{2/3} + \ldots$$

where $\varepsilon_o = 1/(2r_s^2)$ is the kinetic energy of a two-valley equal occupancy state. Thus, for small r_s the difference is positive, in favor of a two-valley state. As r_s increases, $\Delta\varepsilon$ decreases. This indicates the role played by correlations. Note that the above r_s dependent term comes from the second leading term of the correlation energy. The first order exchange and the first leading term of the correlation energy are both cancelled out in the difference, confirming our statement that the transition is a low density phenomenon.

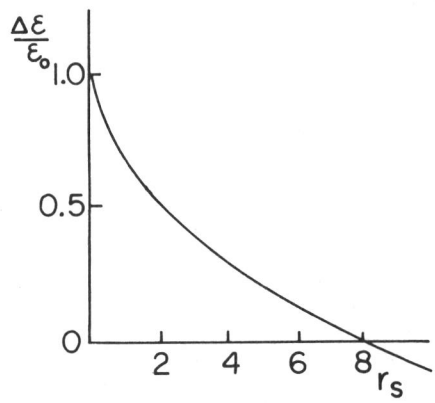

Fig. 2 Energy difference between one- and two-valley states.

For a wide density range, we have performed a numerical evaluation of the energy difference. Figure 2 illustrates the result. As can be seen, the energy difference decreases with increasing r_s and crosses the abscissa at $r_s = 8.011$. At this point, a transition from two- to one-valley states takes

place. In the case of inversion layer electrons with an effective mass 0.2m and average dielectric constant 7.8, this critical r_s corresponds to electron density 1.2×10^{11} cm^{-2}, in good agreement with the data.

Silicon has different valley degeneracies of the ground subbands in different directions. In the [110] direction, there are four equivalent ground subbands, and in the [111] direction, there are six. The lifting of these valley degeneracies may occur also due to electron correlations.

4. Concluding Remarks

We have discussed phase changes which are expected when the density of a two-dimensional electron system is reduced. The ground state energy is continuous throughout, but the system undergoes subtle changes.

Recently, Isihara and Shiwa [9] have found that under a strong magnetic field, which is applied perpendicularly to the surface into which the electrons are confined, the susceptibility shows zigzag changes when plotted against the ratio of the Fermi energy to the field energy. As r_s increases from zero, the slope of the straight lines representing the zigzag changes decreases. Finally, an inversion of the slope takes place at the point where the energy in the absence of a magnetic field vanishes. This inversion of the oscillations seems to be the first sign of the configurational changes of the electrons which are entering a liquid state. This inversion point is around 0.7 in terms of r_s.

The lifting of valley degeneracy at a low density is similar to the case of spin degeneracy. Therefore, when a valley occupancy transition occurs, a domain structure may appear. Moreover, the same mechanism is expected to make a spin polarized state favorable at even lower densities. We have found that $r_s = 13.0$ is the critical point. In other words, at density 4.5×10^{10} cm^{-2} the susceptibility diverges. In a sense, this magnetic phase is similar to the one observed in liquid ^{3}He. Whether or not such a magnetic phase transition takes place before the expected crystallization is a matter to be further investigated. In the absence of a direct experimental evidence, we remark that there is a possible precursor phenomenon. The effective g factor of the electrons in Si inversion layers increases very rapidly towards low densities. This increase has been explained by our related theory very well [10]. The susceptibility anomaly which we have just discussed appears as an extension of the rapid increase.

Acknowledgement

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