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Valley phase transition of a Si inversion layer in high magnetic fields

Ute Gummich* and L. J. Sham
Department of Physics, University of California, San Diego, La Jolla, California 92093
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The change of valley degeneracy in a Si(111) inversion layer due to the intravalley exchange and correlation at high magnetic fields is mapped out as a function of the density and of the strength of the interaction compared with the impurity scattering. The calculated magnetoconductivity is used to explain the observed splitting of the last Landau level in the Shubnikov–de Haas measurements.

I. INTRODUCTION

Rajagopal[1] has pointed out the existence of a ferromagnetic phase when the density of a two-dimensional electron gas is sufficiently low. In the silicon n-channel inversion layer, there are a number of conduction-band valleys equally populated, the number being 2, 4, and 6 for the (100), (110), and (111) surfaces, respectively. Bloss, Sham, and Vinter[2] have shown that, at low densities, the valley degeneracy may be lifted, and have used this state to explain a number of electronic properties of the inversion layer at low densities. The physical reason for the uneven occupation of the conduction valleys is the same as for the ferromagnetic phase: The intravalley exchange and correlation energy that dominates over the kinetic energy at low densities favors the concentration of electrons in fewer valleys.

From qualitative considerations of the Landau levels when a magnetic field is applied normal to the interface, Bloss *et al.*[2] predicted the appearance of additional Landau levels (and, hence, additional Shubnikov–de Haas oscillations) at low densities. An earlier observation[3] was interpreted as the experimental evidence for this. A more direct confirmation is the observation by Englert, Tsui, and Landwehr[4] of an additional splitting of the lowest Landau level in the Shubnikov–de Haas oscillations in an n-channel inversion layer on Si(111) surface. Since the spin splitting in the high magnetic field has already been accounted for, the additional splitting, which only occurs at low densities, is interpreted as the valley splitting. Since on the Si(111) surface, the six conduction valleys are projected onto different wave vectors parallel to the interface, there is no apparent valley splitting due to the surface-scattering mechanism[5] and only the intravalley exchange and correlation effect remains as the responsible mechanism.

The valley splitting of the lowest Landau level is observed not only in samples that have sixfold valley degeneracy in the ground state at high densities, but also in samples with twofold valley degeneracy. There are many explanations for the occurrence of the twofold degeneracy at normal densities.[6] The origin of the reduction from sixfold to twofold degeneracy does not concern us here.

We report here a study of the effects of intravalley exchange and correlation in the presence of a high magnetic field. We restrict our attention to the limit of such a high magnetic field and low density that only the lowest spin-split Landau level is occupied and that excitation to higher levels may be neglected. The phase transition due to the change of the valley degeneracy in the lowest Landau level as a function of the fractional occupation of the Landau level is investigated. For simplicity, the model system is limited to having two conduction valleys. The Landau level has a finite width due to electron-impurity scatterings, included in a simple self-consistent Born approximation.

The phase transition is determined by the competition at a density of the kinetic energy, characterized by the Landau level width Γ due to impurity scatterings and the exchange and correlation energy, characterized by the size of the Coulomb interaction α. The density N is measured as $\nu = N/D$, the fractional occupation of the Landau level, D being the single-spin and single-valley density of states in each Landau level eB/hc. The phase diagram in γ ($\equiv \Gamma/\alpha$) vs ν plane is first calculated in the Hartree-Fock approximation. Correlation correction is calculated in the random-phase approximation (RPA)–plasmon-pole approximation and is found not to change the phase boundaries qualita-

tively. At a physically reasonable value of γ, the system changes from a two-valley degeneracy to one valley as the occupation number ν increases from zero. Since with our approximations, the phase diagram is symmetric about the half-filled case $\nu=1$ there is a one-to-two valley transition as ν approaches 2, the full limit.

The static magnetoconductivity is calculated for a fixed value of γ as a function of the density ν. The density dependence reflects the two-peak structure of the density of states due to the removal of the two-valley degeneracy in the appropriate region of the phase diagram. This explains the observation of Ref. 4. In addition, the calculation shows structures in each peak due to the two-valley to one-valley transition.

In this paper, the possibility of Wigner lattice or charge-density-wave (CDW) formation is ignored. Investigation of CDW formation by Yoshioka and Fukuyama[7] also shows the occurrence of the valley splitting.

II. A MODEL FOR THE INVERSION LAYER

Let the magnetic field $\vec{B}$ be along the z axis normal to the interface of the inversion layer. As a basis set, we choose the wave functions of the form

$$\psi_{kv}(\vec{r})=e^{iky}\varphi(x-X)\zeta(z) . \tag{2.1}$$

The motion of the electron normal to the interface, being confined on the one side by the insulator barrier and on the other by the gate voltage, is quantized and is represented in the lowest subband by $\zeta(z)$, with the quantum number understood, since, in the density range of interest in Si, only the lowest subband is occupied. For the motion in the x-y plane, the Landau gauge is used and the states in the lowest Landau level have wave functions as functions of x and y of the form given by Eq. (2.1), with k being the wave vector of the plane wave in the y direction and $\varphi(x)$, the ground-state harmonic-oscillator wave function. The Landau-level number and spin-up state are also understood since we are concerned only with the lowest spin-split Landau level. The harmonic-oscillator wave function is centered at

$$X=kR^2\equiv k\hbar c/eB , \tag{2.2}$$

R being the cyclotron radius. The only two quantum numbers of interest are k and the valley index v.

The Hamiltonian for these electrons consists of three parts:

$$H=H_0+H_i+H_c . \tag{2.3}$$

H_0 is the total electron energy in the lowest Landau level, given by

$$H_0=\sum_{k,v}\epsilon_0 a^\dagger_{kv}a_{kv} , \tag{2.4}$$

where a_{kv} is the annihilation operator of the state k,v given by Eq. (2.1) and ϵ_0 is the lowest Landau-level energy, independent of wave vector k and valley v. H_i denotes the intravalley electron-impurity scattering:

$$H_i=\sum_{k,k',v}V^{(i)}_{k,k'}a^\dagger_{kv}a_{k'v} . \tag{2.5}$$

H_c denotes the electron-electron interaction that conserves the valley index,

$$H_c=\tfrac{1}{2}\sum_{\substack{k_1,k_1',k_2,k_2',\\ v_1,v_2}} V(k_1,k_1';k_2,k_2')a^\dagger_{k_1v_1}a^\dagger_{k_2v_2}\times a_{k_2'v_2}a_{k_1'v_1} , \tag{2.6}$$

where the Coulomb matrix element is given by

$$V(k_1,k_1';k_2,k_2')=\int d^3r\int d^3r'\psi^*_{k_1v_1}(\vec{r})\psi_{k_1'v_1}(\vec{r})(e^2/|\vec{r}-\vec{r}'|)\psi^*_{k_2v_2}(\vec{r}')\psi_{k_2'v_2}(\vec{r}') . \tag{2.7}$$

The Coulomb interaction between electrons in different valleys is kept but the Coulomb and impurity scatterings that transfer an electron from one valley to another are neglected. This is the same approximation as adopted in Ref. 2.

III. THE VALLEY PHASE TRANSITION

In this section, we consider the valley degeneracy of the ground state in the Hartree-Fock approximation for the electron-electron interaction and the self-consistent Born approximation for the impurity scattering,[8,9] as shown diagrammatically in Fig. 1. Thus the one-electron self-energy term due to the impurity scatterings is[9]

$$\Sigma^i_v(z)=\tfrac{1}{4}\Gamma^2G_v(z) , \tag{3.1}$$

where Γ^2 is the square of the impurity-scattering matrix element in Eq. (2.5) averaged over the impurity configuration[9] of the order $\hbar^2\omega_c/\tau$, ω_c being the cyclotron frequency, and τ the impurity-

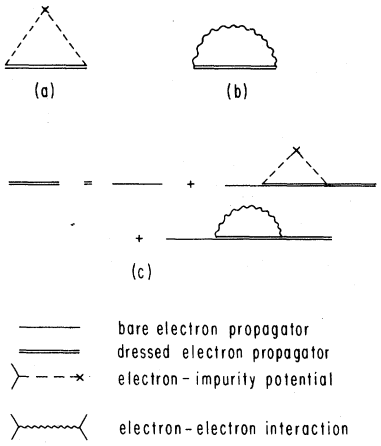

FIG. 1. (a) Impurity contribution to the self-energy. (b) Hartree-Fock contribution to the self-energy. (c) The Dyson equation for the electron propagator.

scattering time. $G_v(z)$ is the dressed one-electron Green's function in valley v.

The self-energy due to the electron-electron interaction in the Hartree-Fock approximation is given by

$$\Sigma_v^x = -\alpha n_v \ , \tag{3.2}$$

where α is the average Coulomb matrix element

$$\alpha = \sum_{k_1,k_2} V(k_1,k_2;k_2,k_1) \tag{3.3}$$

and n_v is the occupation of a Landau level in valley v and thus, in a model of only one Landau level, the density in valley v,

$$n_v = -\pi^{-1} \int_{-\infty}^{\infty} dE\, f(E) \mathrm{Im} G_v(E) \ , \tag{3.4}$$

f being the Fermi distribution function at zero temperature.

The Dyson equation (Fig. 1) reduces to a quadratic equation,

$$G_v(z) = (2/\Gamma^2)\{ (z - \epsilon_0 - \Sigma_v^x) - [(z - \epsilon_0 - \Sigma_v^x)^2 - \Gamma^2]^{1/2} \} \ . \tag{3.5}$$

We have allowed the electron energy in each valley and, hence the valley occupation n_v to be unequal. Equation (3.5) then yields different single-particle spectra for the two valleys but it is insufficient to determine the valley occupation numbers n_v. To do that, we minimize the total energy with the total number of electrons fixed,

$$E = \sum_v [(\epsilon_0 - \tfrac{1}{2}\alpha n_v) n_v - (2\Gamma/3\pi)(1 - \tilde{\epsilon}_v^2)^{3/2}](L^2/2\pi R^2) \ , \tag{3.6}$$

with

$$n_v = \left[\tilde{\epsilon}_v (1 - \tilde{\epsilon}_v^2)^{1/2} + \frac{\pi}{2} + \sin^{-1} \tilde{\epsilon}_v \right] \Big/ \pi \ , \tag{3.7}$$

and

$$\tilde{\epsilon}_v = (\epsilon_F - \epsilon_0 + \alpha n_v)/\Gamma \ , \tag{3.8}$$

ϵ_F being the Fermi energy.

There are only two types of solutions. Depending on the values of the energy ratio γ ($=\Gamma/\alpha$) and the fractional occupation ν ($=N/D$), the electrons are either confined to one valley or distributed equally in both valleys. In the two-valley case, the minimization is simplest to carry out by expressing the total energy in terms of the energy difference of the valley minima in units of Γ, $\tilde{\epsilon}_1 - \tilde{\epsilon}_2 = \Delta$. Then it can be shown from the expression that the lowest energy is either at $\Delta = 0$ or $\Delta = 1 + \tilde{\epsilon}_1$, which means $n_1 = n_2$ or $n_2 = 0$, respectively. We have also numerically verified the conclusion by plotting the total energy versus n_1 for a set of values of γ and ν sufficient to generate the phase boundary in Fig. 2.

The solid curve in Fig. 2 shows the phase diagram of the two phases for an idealized two-dimensional electron system. A qualitative understanding of the condition for each phase may be gained from the total energy expression (3.6). If the positive kinetic energy dominates, the total energy is minimized by spreading the valley occupation n_v evenly over both valleys. If the negative exchange-energy term dominates, the total energy is lowered if one valley gets all the electrons. Thus, when the impurity broadening is small compared with the

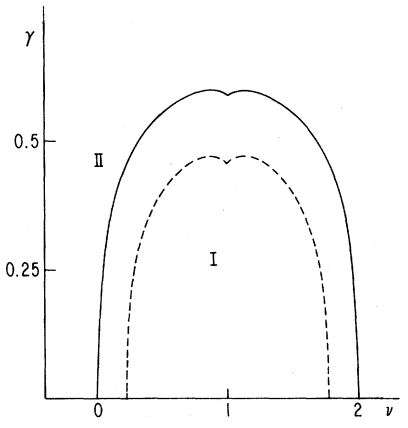

FIG. 2. Phase diagram in Γ/α vs ν plane at $T=0$ K. I denotes the single-valley phase and II the double-valley phase. Solid line is the phase boundary in the Hartree-Fock approximation. Dashed line is when correlation is added.

electron-electron interaction (γ small), the one-valley phase occurs almost in the whole density range $0 \leq \nu \leq 2$. When Γ and α are comparable, the low-density regime for electrons (ν small) or for holes (ν close to 2) favors the kinetic energy term and, hence, the double-valley phase. When the density for the electrons (or holes) is increased, according to (3.6), the exchange energy increases more rapidly than the kinetic energy and the transition from double valley to single valley occurs. This density dependence of the phases in a high magnetic field is just the opposite of the zero-field case where, at low densities, the dominance of the exchange energy favors the single-valley phase and where, at high densities, the double-valley phase takes over.[2] The small dip of the phase boundary at $\nu=1$ and large Γ/α appears not to be a result of the rapidly varying square-root density of states since a Gaussian density-of-states distribution[10] leads to the same feature.

IV. EFFECT ON THE MAGNETOCONDUCTIVITY

Based on the model used to derive the phase diagram in Fig. 2, the static magnetoconductivity is calculated at $T=0$, using the formula[11,9]

$$\sigma_{xx}=(e^2/2\hbar\pi^2)\sum_{v}\int dE\, f(E)[\mathrm{Im}G_v(E)]^2/\{[\mathrm{Im}G_v(E)]^2+[\mathrm{Re}G_v(E)]^2\}\ . \tag{4.1}$$

For the short-ranged impurity scattering, the vertex correction is negligible. Figure 3 shows σ_{xx} vs ν for three different values of γ. The sharp change of σ_{xx}, when the system undergoes the transition from the double-valley phase to the single-valley phase or vice versa, is noticeable only when Γ/α is large. The dip of the conductivity at $\nu=1$ due to the single-valley phase effectively gives the conductivity a two-peak appearance, which occurs at all values of Γ/α.

With this result, we are able to explain qualitatively the observation of the Shubnikov–de Haas peaks at high magnetic fields by Englert *et al.*[4] Where one would expect the lowest Landau level for two-valley or

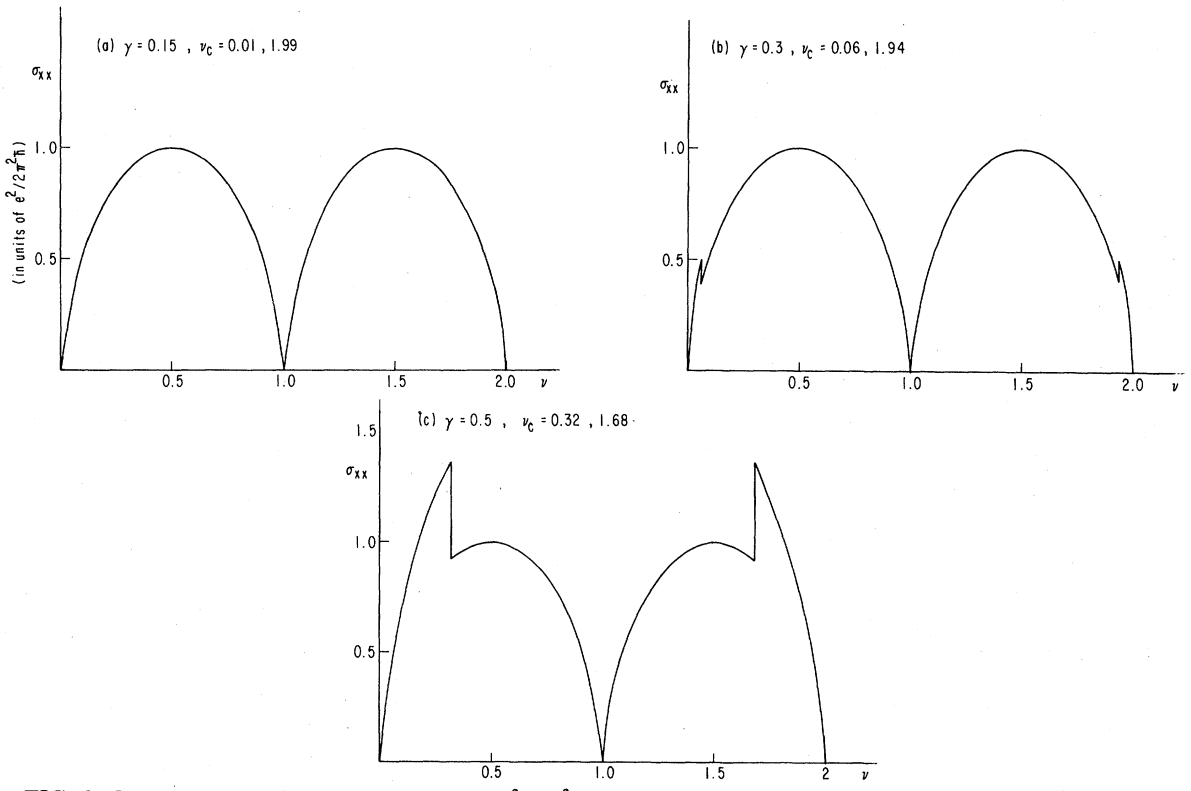

FIG. 3. Magnetoconductivity σ_{xx} (in units of $e^2/2\pi^2\hbar$) vs Landau-level occupation ν for three different values of γ, the ratio of impurity to electron interaction. ν_c is where the phase transition occurs.

six-valley degeneracy, two peaks are observed. For the samples measured, the width of the Landau level Γ is about 3—4 meV. Thus γ ($=\Gamma/\alpha$) is about 0.2. The double- to single-valley transitions occur close to $\nu=0$ and $\nu=2$. The discontinuity in σ_{xx} at the phase transition is too small to be observable [see Fig. 3(a)] and only the two-peak structure is seen.

V. EFFECT OF CORRELATION ON THE PHASE DIAGRAM

At zero magnetic field, the correlation-energy term tends to reduce the effect of the exchange energy.[2] In this section, we examine the effect of correlation in RPA.[12] We take the zero-temperature limit $T\rightarrow 0$ of the coupling-constant integral

$$F_c=-(T/2)\sum_{q,v,n}\int_0^1 d\lambda\,\lambda[v(q)\Pi_v(q,i\omega_n)]^2/[1-\lambda v(q)\Pi_v(q,i\omega_n)]\ , \tag{5.1}$$

where $v(q)$ is the Fourier transform of the Coulomb potential. The proper polarization part is given by

$$\Pi_v(q,i\omega)=-T\sum_{p,E}G_v(p,iE)G_v(p+q,iE+i\omega)\gamma_v(p+q,iE+i\omega;p,iE)\ , \tag{5.2}$$

with the vertex part due to the impurity scattering,

$$\gamma_v(p+q,iE+\omega;p,iE)=1+(\Gamma^2/4)\sum_{p'}G_v(p'+q,iE+i\omega)G_v(p',iE)\gamma_v(p'+q,iE+i\omega;p',iE)\ . \tag{5.3}$$

We have again restricted the electrons to the lowest spin-split Landau level.

Equation (5.3) is solved, yielding

$$\Pi_v(q,i\omega)=-T\sum_{E,k,k'}|\langle k,v\,|\,e^{i\vec{q}\cdot\vec{r}}\,|\,k',v\rangle|^2G_v(iE+i\omega)G_v(iE)\times\left[1-(\pi\Gamma^2R^2/2L^2)\sum_{k,k'}|\langle k,v\,|\,e^{i\vec{q}\cdot\vec{r}}\,|\,k,'v\rangle|^2G_v(iE+i\omega)G_v(iE)\right]^{-1}\ . \tag{5.4}$$

The evaluation of the coupling-constant integral (5.1) with this polarization expression is rather complex and we adopt the plasmon-pole approximation[13] and extend it to high magnetic fields. The polarization is given then approximately by

$$\Pi_v(q,i\omega)=\Pi_v(q,\infty)/[\omega^2/\Gamma^2+\Pi_v(q,\infty)/\Pi_v(q,0)]\ , \tag{5.5}$$

where $\Pi_v(q,\infty)$ and $\Pi_v(q,0)$ are the limiting expressions of (5.4) for $\omega/\Gamma\gg$ and $\ll 1$, respectively. $\Pi_v(q,\infty)$ is of the order q^2 for small q and decays exponentially for large q. $\Pi_v(q,0)$ tends to a constant for small q and also decays exponentially for large q. In this approximation, (5.1) becomes

$$E_c=-(\Gamma D/2)\sum_v\int_0^\infty dx[\Pi_v(x,\infty)/\Pi_v(x,0)]^{1/2}\{1-[1+v(x)\Pi_v(x,0)]^{1/2}\}^2\ . \tag{5.6}$$

When the correlation energy is included, the phase boundary is shown by the dashed curve in Fig. 2. Since the correlation term reduces the effect of the exchange term, the phase boundary is lowered in γ for a fixed occupation ν. There is, however, no qualitative change. The dip at $\nu=1$ remains, for example. The explanation of observations given in the preceding section stands.

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*Permanent address: Institut für Theoretische Physik, Universität zu Köln, D-5000 Köln, Federal Republic of Germany.

[1]A. K. Rajagopal, Solid State Commun. 21, 483 (1977).
[2]W. L. Bloss, L. J. Sham, and B. Vinter, Phys. Rev. Lett. 43, 1529 (1979).
[3]A. A. Lakhani and P. J. Stiles, Solid State Commun. 16, 993 (1975).
[4]Th. Englert, D. C. Tsui, and G. Landwehr, Solid State Commun. 33, 1167 (1980).

[5]L. J. Sham and M. Nakayama, Phys. Rev. B 20, 734 (1979).
[6]M. J. Kelly and L. M. Falicov, Phys. Rev. Lett. 37, 1021 (1976); D. C. Tsui and G. Kaminsky, Solid State Commun. 20, 93 (1976); Phys. Rev. Lett. 42, 595 (1979); B. Vinter and A. Overhauser, *ibid.* 44, 47 (1980); W. L. Bloss, S. C. Ying, and J. J. Quinn, Phys. Rev. B 23, 1839 (1981).
[7]D. Yoshioka and H. Fukuyama (unpublished).
[8]R. Kubo, S. J. Miyake, and N. Hashitsume, in *Solid State Physics,* edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1965), Vol. 17, p. 270.
[9]T. Ando and Y. Uemura, J. Phys. Soc. Jpn. 36, 959 (1974).
[10]T. Ando, J. Phys. Soc. Jpn. 37, 622 (1974).
[11]W. Götze and J. Hajdu, Solid State Commun. 29, 89 (1978).
[12]T. Ando and Y. Uemura, J. Phys. Soc. Jpn. 37, 1044 (1974).
[13]B. I. Lundqvist, Phys. Kondens. Mater. 6, 206 (1967); A. W. Overhauser, Phys. Rev. B 3, 1888 (1971).