Staging transitions in multiple-quantum-well systems

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We suggest the possibility that staging transitions, similar to those in graphite intercalation compounds, might occur in a strong magnetic field for high-quality modulation-doped multiple-quantum-well systems with sufficiently low carrier density, $\bar{\rho}$, and sufficiently short superlattice period, d. In a stage-n state electrons would occupy every nth quantum well. A simple model calculation suggests that $n \geq 1$ states have lower energy for $d^3\bar{\rho} \lesssim 0.3$.

Graphite intercalation compounds[1,2] with low intercalant atom concentrations form structures in which there are n carbon layers between each layer of intercalant atoms. These structures are referred to as stage-n compounds and staging transitions occur between the different structures in which n decreases as the intercalant atom concentration increases. The staging transitions result from an attractive effective intercalant-intercalant interaction for atoms in the same plane and a repulsive interaction between intercalants in different planes.[3-5] We suggest here that similar phenomena might occur for a multiple-quantum-well (MQW) structure in a magnetic field sufficiently strong that the electrons in each two-dimensional electron gas (2D EG) layer are in the lowest Landau level. In a MQW, regions of one semiconductor (typically GaAs) are separated by regions of a higher band-gap semiconductor (typically $Ga_{1-x}Al_xAs$) which act as barriers separating quantum wells. The role of the intercalant atoms, in this case, is played by the electrons and the role of the galleries between carbon layers is played by the quantum wells. The attractive interaction which can drive the staging transition is the exchange interaction between electrons in the same quantum well. The repulsive interaction is the Coulombic interaction between charged planes, which increases with their separation, so that the staging transition occurs at higher electron density for shorter superlattice period. The strong magnetic field is necessary to create Landau levels which have a degeneracy sufficient to accommodate an areal density up to

$$\sigma_1 = eB/hc \simeq 0.24\times 10^{11} B(\text{tesla})\ \text{cm}^{-2} \tag{1}$$

in each quantum well, without any increase in the kinetic energy per electron.

We refer to a state in which electrons occupy only every nth quantum well as a stage-n state. In order to estimate the density below which $n \geq 1$ states have lower energy, we adopt the simplified model of periodically arranged quantum wells with vanishing thickness separated by a distance d (the superlattice period) and assume that tunneling between different 2D EG layers may be neglected. This is the model used, for example, to study plasmons in MQW systems[6-8] and, in that case at least, it gives good agreement with experiment.[9,10] The Coulomb energy of this system is

$$E_c = \frac{e^2}{2\epsilon}\int d\mathbf{r}\int d\mathbf{r}\frac{[\rho(\mathbf{r})-\rho_I(\mathbf{r})][\rho(\mathbf{r}')-\rho_I(\mathbf{r}')]}{|\mathbf{r}-\mathbf{r}'|}$$
$$= \frac{e^2}{L_xL_yL_z}\sum_{q_z}{}' \frac{2\pi}{\epsilon q_z^2}|\rho(q_z)-\rho_I(q_z)|^2 , \tag{2}$$

where L_x, L_y, and L_z are the lengths of the system in the x, y, and z directions, ϵ is the dielectric constant, $\rho(\mathbf{r})$ is the electron number density $\rho_I(\mathbf{r})$ is the number density of the neutralizing ionized donors required by the long range of the Coulomb interaction, and we have assumed that $\rho(\mathbf{r})$ and $\rho_I(\mathbf{r})$ depend only on the coordinate perpendicular to the 2D EG layers, which we take to be the z coordinate. For a stage-n-state every nth quantum well has a 2D EG with areal density $\sigma = nd\bar{\rho}$ where $\bar{\rho}$ is the mean electron density. It follows that

$$\rho(q_z) = \rho L_xL_yL_z \sum_i \delta(q_z, 2\pi i/dn) . \tag{3}$$

Assuming the ionized donor density to have the periodicity of the MQW and defining f_k by

$$\rho_I(q_z) = \rho\bar{L}_xL_yL_z \sum_k f_k \delta(q_z, 2\pi k/d) \tag{4}$$

gives

$$\epsilon_c \equiv \frac{E_c}{N}$$
$$= \frac{\bar{\rho}e^2n^2d^2}{\pi}\left[\sum_{i=1}^{\infty}\frac{1}{i^2} + \frac{1}{n^2}\sum_{k=1}^{\infty}\frac{|f_k|^2 - f_k - f_{-k}^*}{k^2}\right] . \tag{5}$$

The second term in the large parentheses in Eq. (5) gives a contribution to ϵ_c which is independent of n, so that the distribution of ionized donors is irrelevant in determining the stage number. For the sake of definiteness we assume that the ionized donors are distributed in a narrow layer midway between 2D EG layers, in which case $f_k = (-1)^k$. Then the sums in Eq. (5) are known and we obtain

$$\frac{\epsilon_c}{e^2/\epsilon d}=\frac{\bar{\rho}d^3\pi}{6}(n^2+2)\,. \tag{6}$$

The Coulomb interaction favors the $n=1$ state in order to obtain as uniform a charge density as possible. However, exchange and correlation effects of the electrons within a given 2D EG layer give a negative contribution to the energy per electron which increases in magnitude as the density increases and the electron moves closer to its exchange correlation hole. For electrons in the lowest Landau level of a 2D EG this energy is quite accurately known.[11-14] For $\sigma=nd\bar{\rho}\ll\sigma_1$ the electrons are expected to form a Wigner crystal.[13,15] In this limit which (in the interests of simplicity) we assume to apply, the exchange and correlation energy per electron reduces to the Madelung energy of the 2D Wigner crystal[16] so that

$$\frac{\epsilon_{xc}}{e^2/\epsilon d}=-1.9605(\bar{\rho}nd^3)^{1/2}\,. \tag{7}$$

In higher-stage states the electron density in occupied 2D EG layers is higher and the exchange-correlation interaction increases in strength. Since ϵ_{xc} in $e^2/\epsilon d$ units is proportional to $(\bar{\rho}d^3)^{1/2}$ while ϵ_c is proportional to $\bar{\rho}d^3$ higher-stage states will always be favored at low electron densities provided that the magnetic field is strong enough that they can be formed without occupying higher Landau levels.

Combining Eq. (5) and Eq. (7) we estimate the transition from stage-n to stage-$n+1$ states occurs for

$$\bar{\rho}d^3\simeq 14\left[\frac{\sqrt{n+1}-\sqrt{n}}{2n+1}\right]^2 \tag{8}$$

provided that $\nu\equiv n\bar{\rho}d/\sigma_1\lesssim 1$. In Fig. (1) we plot $\epsilon\equiv\epsilon_c+\epsilon_{xc}$ for the lowest energy stage-n state and

$$\mu=\frac{d}{d\bar{\rho}}(\bar{\rho}\epsilon)=\frac{e^2}{\epsilon d}\left[\frac{\bar{\rho}d^3\pi(n^2+2)}{3}-2.9408(\bar{\rho}nd^3)^{1/2}\right] \tag{9}$$

in units of $e^2/\epsilon d$ versus $\bar{\rho}d^3$ for a realistic range of values. For example, a MQW system with $\bar{\rho}=10^{17}$ cm^{-3} and $d=10$ nm has $\bar{\rho}d^3=10^{-1}$ and $\bar{\rho}d/\sigma_1=4.136/B$(tesla).

Our emphasis on strong fields is not meant to imply that similar phenomena could not occur at weaker or zero fields and results from our estimate that stage-n states could be realized more easily in strong fields. At zero field the energy per electron for a stage-n state is given approximately by[17]

$$\epsilon=\frac{e^2}{\epsilon d}\left[\frac{\bar{\rho}d^3\pi}{6}(n^2+2)+\frac{\bar{\rho}d^3\pi n}{2}\frac{a_0^*}{d}-1.06(\bar{\rho}nd^3)^{1/2}\right], \tag{10}$$

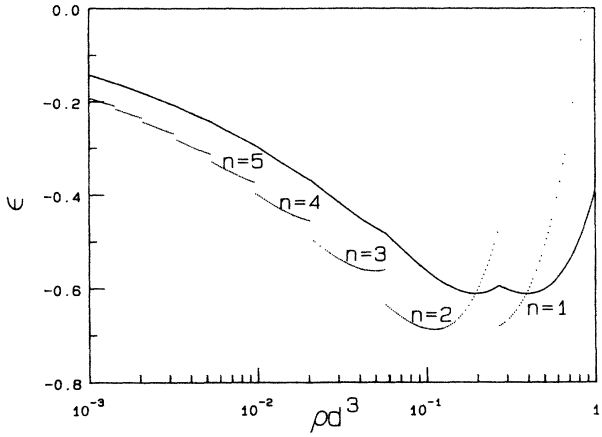

FIG. 1. Energy per electron, ϵ, and chemical potential, μ, in units of $e^2/\epsilon d$ vs $\bar{\rho}d^3$. The solid line (ϵ) is continuous while the dotted line (μ) is discontinuous at each staging transition.

where the first term is the electrostatic energy, the second term is the kinetic energy per electron for motion within the quantum wells, and the third term is the exchange energy. In the second term $a_0^*\propto 1/m^*$ is the semiconductor's Bohr radius (~ 10 nm for GaAs). Note that the kinetic energy opposes staging transitions and that the exchange interaction, which favors staging, is weaker than in the strong-field case. From Eq. (10) we estimate that the transition from stage-n to stage-$n+1$ states at zero field occurs for

$$\bar{\rho}d^3=4.1\left[\frac{\sqrt{n+1}-\sqrt{n}}{2n+1+(a_0^*/d)}\right]^2. \tag{11}$$

For $a_0^*=d$ the $n\geq 1$ states have lower energy for $\bar{\rho}d^3\lesssim 2\times 10^{-2}$ compared to the condition $\bar{\rho}d^3\lesssim 0.3$ which holds for the strong-field case.

The Landau-level broadening expected from the ionized donors and other sources in real MQW systems will lift the Landau-level degeneracy assumed here and should be kept to a minimum by modulation doping and using high-quality samples if $n\geq 1$ states are to occur. In addition, our neglect of interlayer tunneling and the finite thickness of the 2D EG layers may result in an overestimate of the transition densities, especially as d becomes shorter. Nevertheless, the results presented here suggest that $n\geq 1$ states should be realizable in practice. A stage-n state could be identified by using the fractional quantum Hall effect[18] to measure the areal density of the 2D EG layers. Assuming independent conduction in each 2D EG layer,[19,20] minima in the magnetoresistance should occur when $\nu\equiv nd\rho\sigma_1$ is a fraction with an odd denominator and especially when $\nu=\frac{1}{3}$ or $\nu=\frac{2}{3}$.

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