Oscillating magnetization of quantum-well electrons in a parallel magnetic field

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The magnetization of quasi-two-dimensional electron systems in rectangular quantum wells with magnetic fields parallel to the potential walls is computed from the recently calculated infinite-power-series expansion of the energy eigenvalues. It may be used to determine the band offset. The magnetization oscillates as a function of the chemical potential. This is a consequence of electric and magnetic hybridization of the eigenstates when the cyclotron radius is comparable to the well width. Minima occur whenever the chemical potential crosses the lower edge of a subband. Calculations for a parabolic potential well show the universality of the oscillations in laterally confined systems.

I. INTRODUCTION

Quantum wells in superlattices[1] and *n-i-p-i* structures[2] with magnetic fields **B** parallel to the potential walls have eigenstates characterized by hybrid electrical and magnetic quantization.[3–6] Their energy eigenvalues and wave functions have been computed recently by a new, graph-supported method.[7]

After numerical solutions of the problem have been obtained previously by a number of workers[4,8,9] the full energy spectrum is now available in analytical form. This facilitates the computation of physical effects associated with the density of states and the change of energy with magnetic field. An obvious candidate for closer scrutiny is the magnetization of quantum-well electrons, especially for cases where the cyclotron radius is comparable to or larger than the well width. This complements earlier calculations of Landau[10] and Heuser and Hajdu[11] for electron gases with cyclotron radii much smaller than the dimensions of the confining volume, and of Zawadzki[12] for a two-dimensional electron gas with a magnetic field perpendicular to the potential walls. It is the purpose of this paper to show that the magnetization in a parallel field $\mathbf{B}=\mathbf{e}_y B$ should oscillate as the number of electrons in the well and the chemical potential increase. This new effect is basically due to the fact that with increasing B the energy of states with small momentum $\hbar k_x$ parallel to the potential walls increases whereas the energy of states with large k_x decreases. As a result, in a square-well potential, the change of magnetization is positive when states with large k_x are populated and it is negative when the chemical potential μ moves through states with small k_x. These competing changes cause the magnetization arches of Fig. 1.

II. MAGNETIZATION AND ENERGY EIGENVALUES OF SQUARE WELLS IN PARALLEL FIELDS

The magnetization M of an electron gas at temperature T can be calculated from its thermodynamic potential Ω:

$$M=-\left[\frac{\partial\Omega}{\partial B}\right]_{V,T,\mu=\text{const}}, \tag{1}$$

where Ω is being determined by the energies E_α of single particle states characterized by the set of quantum numbers α,

$$\Omega=-k_B T 2\sum_\alpha \ln\{1+\exp[(\mu-E_\alpha)/k_B T]\}\ . \tag{2}$$

From Eq. (1) it follows that the magnetization M is equal to the average magnetic moment $\langle M\rangle$

$$M=\langle M\rangle\equiv 2\sum_\alpha f_\alpha^0\left[-\frac{\partial E_\alpha}{\partial B}\right], \tag{3}$$

where f_α^0 is the Fermi distribution function.

Let us first consider an electron gas confined to a rectangular quantum well of width L_z. The confining potential $V(z)$ is given by

$$V(z)=\begin{cases}V_0 & \text{for } |z|>L_z/2\\ 0 & \text{for } |z|\le L_z/2\ .\end{cases} \tag{4}$$

A homogeneous magnetic field $\mathbf{B}=\mathbf{e}_y B$ is applied in the y direction. The vector potential is chosen to be $\mathbf{A}=\mathbf{e}_x Bz$. In x and y directions the system is translationally invariant with periodic boundary conditions. In this case the quantum numbers are $\alpha=(n,k_x,k_y)$, the integer n labeling the different energy levels with the same wave numbers k_x,k_y. The energy eigenvalues E_α of this system for $V_0\to\infty$ are[7]

$$E_\alpha=E_n(z_0(k_x),k_y)=\frac{\hbar^2}{2m^*}\left[\frac{b^2 z_0^2}{L_z^4}+k_y^2+\frac{1}{L_z^2}\sum_{r=0}^{\infty}\sum_{t=0}^{\le r/2}G_{n;r,t}\,b^{2r}\left[\frac{z_0}{L_z}\right]^{2t}\right] \tag{5}$$

with $z_0=-\hbar k_x/eB$, $b=BeL_z^2/\hbar$, and m^* the effective electron mass; interactions between spins and field are neglected. The $G_{n;r,t}$ are numerical factors independent of the system parameters.

If the barrier height V_0 is finite but still large enough so that in the barrier the influence of the B field on the wave functions of the lowest lying states can be neglected, one still obtains Eq. (5) for the energy eigenvalues, with the only change that the expansion coefficients $G_{n;r,t}$ become functions $G_{n;r,t}(v)$ of the normalized barrier height $v=2m^*L_z^2V_0/\hbar^2$.[13]

Combining Eqs. (3)–(5) yields the magnetization per unit volume for a rectangular quantum well in a parallel magnetic field:

$$\frac{M}{V}=-\frac{1}{\pi^2}\mu_B\frac{m_0}{m^*}\frac{eB}{\hbar L_z}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}d(k_xL_z)\sum_{r=0}^{\infty}\sum_{t=0}^{r+1}(r+1)G_{n;r+t+1,t}(v)b^{2r}(k_xL_z)^{2t}\int_{-\infty}^{\infty}d(k_yL_z)f_n^0(k_x,k_y)\ , \tag{6}$$

where $\mu_B=e\hbar/2m_0$ and m_0 is the free-electron mass.

III. MAGNETIZATION OSCILLATIONS AND PHYSICAL PICTURE

The de Haas–van Alphen oscillations of the magnetization, which are well known in three-dimensional electron gases and two-dimensional systems with B perpendicular to the potential walls,[12,14,15] would be visible only for extremely strong parallel fields. For fields below 10 T and well widths $L_z<500$ Å, electrical quantization of the hybrid energy levels suppresses the Landau fan, i.e., the energetic distance between levels n and $n+1$ exceeds by far the Landau-level separation. Thus the $M(B)$ curves obtained from Eq. (6) are essentially monotonous functions of small and intermediate, parallel B. However, if one computes the magnetization as a function of the chemical potential μ, i.e., the number of electrons in the quantum well, one obtains Figs. 1(a)–1(c) which exhibit very pronounced oscillations of M.

The magnetization becomes small whenever the Fermi energy crosses the bottom of an energy band $E_n(z_0(k_x),k_y)$ at $k_x=0=k_y$. This behavior can be understood by looking into the dependence of the energy eigenvalues on B and k_x in Eq. (3). For fixed k_x an increase in B results in two competing effects on the energy E_α. The narrowing of the harmonic oscillator potential $(m^*/2)\omega_c^2(z-z_0)^2$, $\omega_c=eB/m^*$, tends to increase the energy, while the decrease in $|z_0|=|\hbar k_x/eB|$ tends to lower the energy, see Fig. 2. For small k_x, i.e., $|z_0|<L_z/2$, the energy gain with B dominates: The leading terms in Eq. (5) are the ones independent of z_0 (for small B the energy is proportional to const$+B^2$). For large k_x the minimum position z_0 of the harmonic oscillator potential superimposed on the quantum well by the parallel B field, will be quite outside the well, and the energy increases strongly with $z_0\sim 1/B$. This result of the numerical evaluation of Eq. (5) is illustrated by Fig. 2. Contributions to the sum in Eq. (3) from the lower (k_x small) and upper (k_x large) parts of an energy band therefore enter with different signs and lead to the arching structures of Fig. 1.

IV. BAND OFFSET, WELL SHAPE, AND SPIN PARAMAGNETISM

Figures 1(a)–1(c) show the influence of the well parameters on the magnetization. The feature of the curves that is most sensitive to changes in the well parameters is

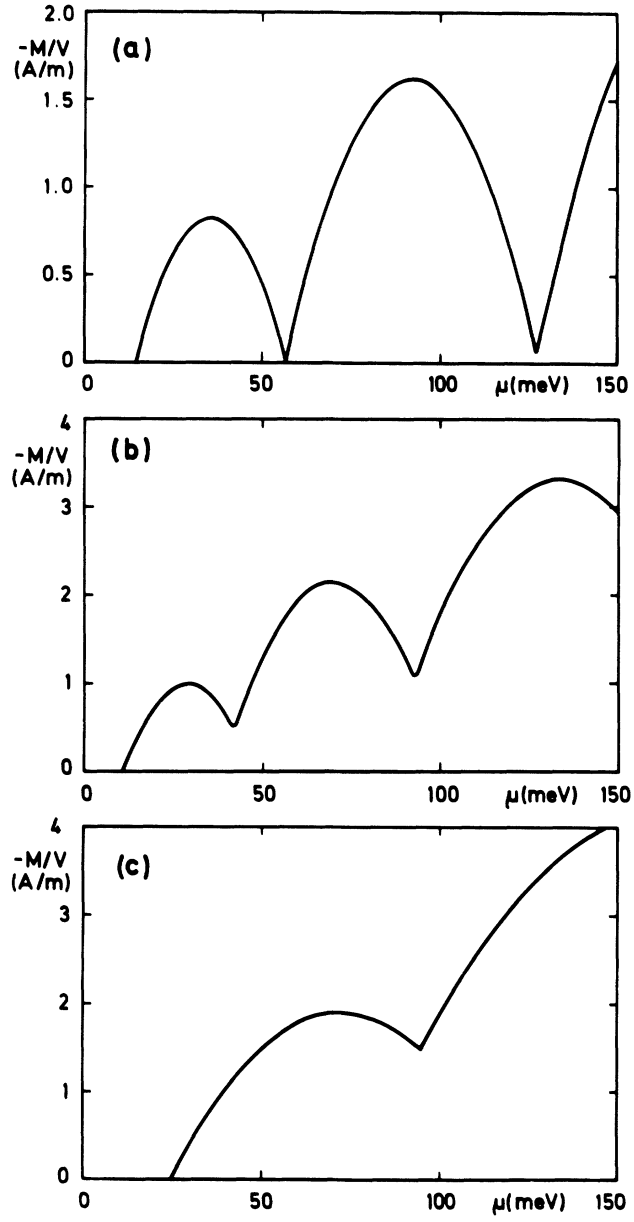

FIG. 1. Negative magnetization $-M/V$ per unit volume as a function of the chemical potential μ for three different rectangular quantum wells at constant magnetic field $B=1$ T ($m^*=0.0665m_0$ as in GaAs): (a) infinite potential well, width $L_z=200$ Å, $T=0$ K; (b) finite potential well, $V_0=228$ meV (corresponding to an $Al_{0.3}Ga_{0.7}As$ barrier), $L_z=200$ Å, $T=4.2$ K; and (c) $V_0=228$ meV, $L_z=120$ Å, $T=0$ K. Note the small temperature effect on the shape of the curves.

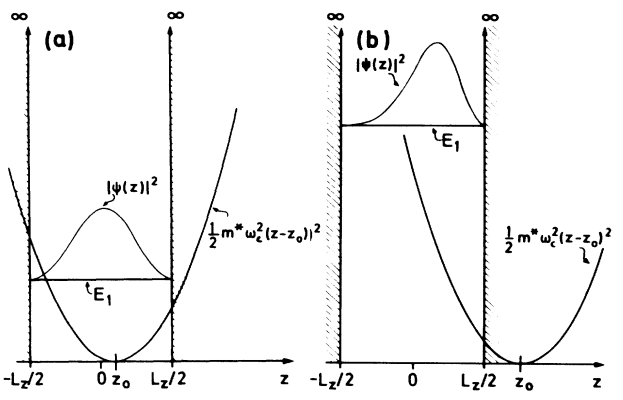

FIG. 2. Infinite potential well, harmonic oscillator potential, and probability density $|\psi(z)|^2$ for two values of $z_0=-\hbar k_x/eB$ (schematic): (a) $z_0=0.1L_z$ and (b) $z_0=0.75L_z$. The horizontal lines indicate the ground-state energies for $k_y=0$: The narrower the region to which the electron wave functions are being confined the higher are the energy eigenvalues.

the ratio of maximum and minimum values of the magnetization. Table I lists the ratios of the first maximum to the first minimum for wells of width 120, 200, and 300 Å and for two different values of the barrier height: $V_0=228$ meV and $V_0=323$ meV, corresponding to conduction-band offsets of 60% and 85%, respectively. The difference in the offset changes the magnetization ratio by about 25%, an effect that should be observable in precision magnetization measurements.[14,15] At $B=5$ T the magnetization changes between the first maximum and the first minimum by 2.5 A/m in a 200-Å well. In a superlattice of 1 cm$\times$1 cm area perpendicular to the growth direction the corresponding change in magnetic flux is 0.3 flux quanta per quantum well. Determination of the offset from experiments will require consideration of the magnetization due to holes, and of the well deformation because of accumulated charge densities. This can be done if the actual system parameters are precisely known.

Just to show that other than square-well potentials also give rise to structures in the magnetization we consider a parabolic potential well $V(z)=m^*\omega_0^2z^2/2$. For the well-known composite harmonic oscillator[5,16,17] the energy levels have been calculated analytically. Inserting the energy eigenvalues

TABLE I. Ratio of the first maximum to the first minimum value of the magnetization for three well widths and band offsets of 60% and 85% and relative difference of these values, calculated for $T=0$ K and $B=1$ T.

Well width	120 Å	200 Å	300 Å
Offset 60%	1.28	2.13	3.33
Offset 85%	1.49	2.64	4.54
Difference	16%	24%	36%

$$E_n(k_x,k_y)=(n+\tfrac{1}{2})\hbar(\omega_c^2+\omega_0^2)^{1/2}+\frac{\hbar^2k_y^2}{2m^*}+\frac{\hbar^2k_x^2}{2m^*}\left[\frac{\omega_0^2}{\omega_c^2+\omega_0^2}\right] \tag{7}$$

into Eq. (3) we obtain for $T=0$:

$$M=-\frac{1}{2\pi}\mu_B\frac{m_0}{m^*}\frac{eB}{\hbar}L_xL_y\left[\frac{\omega_c^2+\omega_0^2}{\omega_0^2}\right]^{1/2}(N+1)\times\{\tfrac{1}{4}-[m-(N+1)]^2\} \tag{8}$$

with $\omega_c=eB/m^*$ and $m=\mu/\hbar(\omega_c^2+\omega_0^2)^{1/2}$; N is the index of the uppermost occupied subband. The plot of the magnetization in Fig. (3) is very similar to the infinite square-well magnetization of Fig. 1(a). We also expect structures in the magnetization of metal-oxide-semiconductor field-effect transistors in parallel B fields when with increasing gate voltage the Fermi level of an inversion layer moves through higher subbands.

Taking into account the spin paramagnetism does not change the overall picture: For $T=0$ and low fields the paramagnetism can be calculated approximately from the density of states of the field free square well of infinite height:

$$D(E)=L_xL_y\frac{m^*}{\pi\hbar^2}\sum_{n=1}^{N}\Theta(E-E_n(0,0)) . \tag{9}$$

The result for the paramagnetic part of the magnetization is then easily obtained:

$$\frac{M_p}{V}=\frac{1}{2\pi}\mu_B\frac{m^*}{m_0}\frac{eB}{\hbar L_z}f(\mu) , \tag{10}$$

where $f(\mu)=N$ for μ between $E_N+\mu_BB$ and $E_{N+1}-\mu_BB$, and $f(\mu)$ rises linearly from $N-1$ to N for μ between $E_N-\mu_BB$ and $E_N+\mu_BB$. This paramagnetism is proportional to (m^*/m_0) while the diamagnetism of Eq. (6) is proportional to (m_0/m^*). The diamagnetic contribution then dominates the paramagnetic contribution by a factor of $(m_0/m^*)^2$ which is of the order of 100 in semiconductors.

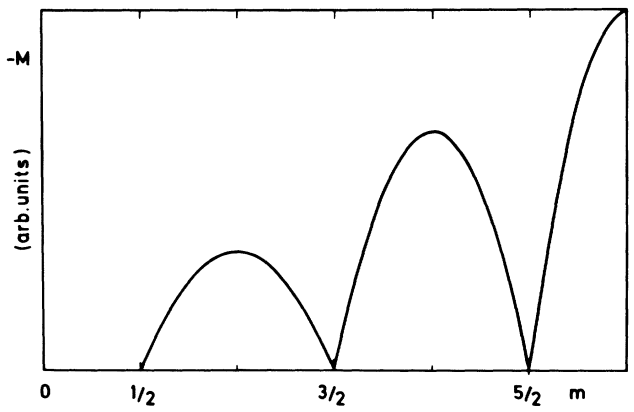

FIG. 3. Negative magnetization $-M$ as a function of the relative chemical potential $m=\mu/\hbar(\omega_c^2+\omega_0^2)^{1/2}$ for a parabolic potential well. $V(z)=m^*\omega_0^2z^2/2$ at constant parallel magnetic field $B=m^*\omega_c/e$ and $T=0$ K.

V. CONCLUSIONS

In order to measure the dependence of the magnetization of a quantum well on the Fermi energy and observe the predicted oscillations, a system is needed in which it is possible to change the number of electrons in the well. This may be done, e.g., by photoexcitation. However, one has to make sure that there is no recombination of the produced electron-hole pairs. This can be achieved if the holes can tunnel out of the hole quantum well into an energetically favorable level that is spatially separated from the electron well. Such a system is realized in a hetero-*n-i-p-i* superlattice, where rectangular quantum wells are situated at the minima of the *n-i-p-i* superlattice potential.[2] Here our method of calculating the oscillating magnetization in conjunction with its measurement should make it possible to determine the band offset.

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