Electron Structure Near Abrupt Edges in 2DEG under Strong Magnetic Field.

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abstract

Energies and wave functions of edge states in two dimensional electron gas are evaluated for a finite step potential barrier model. The spectrum, instead of smooth bending of Landau branches in the vicinity of the barrier acquires a steplike form; unexpected edge plateaus and significant energy gap reduction take place between the neighbouring Landau branches above the barrier tops. The origin of these phenomena is traced. Stability with respect to modifications is established. Manifestation of the qualitatively new features of electron densities of states in abrupt confinements through magnetooptical and nuclear magnetic spin relaxation effects is proposed.

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1 Introduction

Strong magnetic fields and progress in heterostructure quality allowed discovery of such dramatic phenomena in two dimensional electron gas (2DEG) like Integer and Fractional Quantum Hall Effect [?]. In the microscopic theory the edge states, classically represented by electrons skipping in circular segments along the edges, play an important role. Many magnetotransport experiments in two dimensional electron gas have been qualitatively understood recently by means of a simple edge - state model [?]. This model is based on the picture of smooth Landau level bending by the potential formed by external charges. The intersections of each Landau level with the Fermi surface create widely separated narrow edge channels [?].

The semiclassical notion of the Landau level bending, however, is not always applicable to the electronic structure in the vicinity of the barrier representing an edge or an interface (or random potential). It is definitely not valid for potentials with large gradients. In such situations often used quantum mechanical model [?] is limited to the extreme case of an infinite barrier. Recently Chklovskii et al [?], using the self-consistent electrostatic approach, showed that the resulting effective potential should acquire a step-like shape even if the external potential is smooth.

In this paper, finite step potential is considered to better approximate the interface or the steplike potential just mentioned. The electron structure exhibits two rather unexpected phenomena: the edge plateaus and the Lan-
dau gap reduction. These phenomena are not present in either of previously studied models.

The interface might be either a “boundary” confining 2DEG or an interface between two different materials. The finiteness of the barrier confining 2DEG is especially important, if the confinement is realized by means of an interface between two similar materials. Then, in very strong magnetic fields, the magnetic field induced splitting (between Landau levels) may be comparable to the potential barrier height. For example, in the 2DEG formed at the interface between GaAs and GaAl$_{1-x}$As$_x$, the effective interface potential barrier is about 0.3 eV. The Landau level spacing in strongest magnetic fields experimentally available is just a few times smaller. In particular, for the steplike potential with wide steps (on the scale of magnetic length) of height $\hbar\omega_c$ [?, ?], the two quantities are equal.

Two dimensional electron systems are realized at abrupt interfaces between two slightly different semiconductor crystals. Such systems are prepared by molecular beam epitaxy where deposition as well as doping can be controlled on atomic layer level. Lateral confinement within the plane of 2DEG can be achieved in various ways. In one of them, the gate voltage restricts the electron motion. Due to the distances between the gate and the 2DEG plane, the resulting confinement potential is very smooth within the plane. Mesa etched samples in which the surface charge substitutes the gate voltage, fall also into this category of smoothly confined systems. These have
been studied in detail theoretically [?].

Recently, systems with varying chemical composition along the growth plane have been prepared. In such systems the effective confinement barrier height is approximately given by the well studied discontinuity in valence and conduction bands at heterostructures. Moreover, these barriers are localized within just a few interatomic distances. Therefore on a scale of magnetic length, even for strong magnetic fields they represent very abrupt barriers. For such systems our model is appropriate. Systems of this type have been also prepared in a form of very narrow channels (quantum wires). In these systems consequences of interaction between the two opposite edges can be studied.

The paper is organized as follows. In section 2, general properties of confinement barriers are reviewed. In particular, the concept of lagging of the electron center of mass behind the Larmor orbital center, due to the edge, is introduced. Next section is devoted to a rather detailed analysis of the simplest model of an abrupt barrier: the finite rectangular step. Spectrum exhibits two rather unexpected phenomena. Landau branches do not rise steadily towards the edge, but instead develop a series of "edge plateaus". The energy separation between the Landau branches does not remain constant: at certain regions within the edge it gets significantly reduced compared to $\hbar \omega_c$. Both of these phenomena are peculiar to finite abrupt edge barriers and do not exist in smoothly confined systems. In section 4, some ex-
periments in which the characteristically modified electron densities of states should be observable like nuclear magnetic spin resonance and magnetooptics are discussed. The stability of results obtained for the simple model is examined in section 5.

2 General description of the edge.

Here, we consider a system of 2D noninteracting electrons in the vicinity of a boundary under the homogeneous magnetic field \( B \) perpendicular to the \( xy \)-plane. The edge or interface is described by a potential barrier \( V(x) \).

The one particle Hamiltonian is

\[
H = \frac{1}{2m} (\vec{p} - \frac{e}{c} \vec{A})^2 + V(x).
\tag{1}
\]

where \( \vec{A}(x) \) is the vector potential describing the applied magnetic field. In the Landau gauge, \( \vec{A} \equiv (0, Bx, 0) \), the motion along the \( y \)-direction is free and we can separate variables:

\[
\psi_{n,X}(x,y) = \frac{1}{\sqrt{2\pi}} \exp \left( \frac{iXy}{l^2} \right) \phi_{n,X}(x).
\tag{2}
\]

The wave function \( \phi_{n,X}(x) \) obeys the one dimensional Schrödinger equation:

\[
\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega_c^2 (x - X)^2 + V(x) \right] \phi_{n,X}(x) = E_n(X) \phi_{n,X}(x) \tag{3}
\]

where \( l \equiv \sqrt{\frac{\hbar}{eB}} \) is the magnetic length, \( \omega_c \equiv \frac{eB}{mc} \) is the cyclotron frequency and \( X \) is coordinate of the center of a Larmor orbit. This is the Schrödinger
equation for the harmonic oscillator superimposed with the barrier. The integer \( n \) parametrizes discrete Landau levels, \( n = 0, 1, 2, \ldots \).

If the barrier \( V(x) \) is a smooth function of \( x \) (so that the force \( \frac{\partial V(x)}{\partial x} \) is small compared to \( \hbar \omega_c/l \)), then all the Landau levels follow the potential:

\[
E_n(X) = \left( n + \frac{1}{2} \right) \hbar \omega_c + V(X) \tag{4}
\]

In this case the spacing between different Landau branches always remains a multiple of \( \hbar \omega_c \).

In another extreme case of an infinite step barrier, simple boundary condition of vanishing of the wave function is to be imposed: \( \phi_{n,X}(0) = 0 \). It was studied by McDonald and Středa [?], who obtained energies of first few levels as a function of the distance \( X \). Deep inside the region to the left of the barrier \( (X << 0) \) the influence of the interface is negligible and \( E(X) \rightarrow \hbar \omega_c \left( n + \frac{1}{2} \right) \). As \( X \) approaches the barrier, the energy levels rise due to repulsive effect of the infinite barrier. For orbits centered in the "forbidden" region to the right of the barrier, the energies continue to rise indefinitely.

Certain general statements about the electron structure can be made without specifying the shape of the confinement barrier \( V(x) \). The Hamiltonian of the 1D Schrödinger equation depends on \( X \). The Hellmann - Feynman theorem [?] applied to \( X \) as a parameter provides the following useful relation.
which is independent of the barrier profile:

\[
\frac{dE_n(X)}{dX} = <\phi_{nX}|\frac{dH_X}{dX}|\phi_{nX}> = m\omega_c^2 <\phi_{nX}|X-x|\phi_{nX}>
\]  \hspace{1cm} (5)

An important quantity \(X - \bar{x}\), where \(\bar{x}\) is the average electron position, will be referred to as a displacement of the classical Larmor orbit center due to repulsion by the barrier. The displacement therefore becomes:

\[
X - \bar{x} = \frac{1}{m\omega_c^2} \frac{dE_n(X)}{dX}
\]  \hspace{1cm} (6)

The center of mass \(\bar{x}\) characterizing the wave function \(\phi_{nX}(x)\) is thus easily obtained by differentiating the dispersion relation \(E_n(X)\). It is clear, that far from the barrier, \(x << X\), the displacement is zero, and \(X = \bar{x}\). When the Larmor orbital center \(X\) approaches the barrier, its repulsion gives rise to lagging of \(\bar{x}\) behind \(X\). For the infinite confinement barrier, lagging of \(\bar{x}\) behind its Larmor orbit’s center \(X\) steadily increases as \(X\) grows (the wave function is nonzero for \(x<0\) only).

For any monotonously rising potential the function \(E_n(X)\) is monotonous in \(X\). In the particular case of the finite step barrier, \(\bar{x}\) laggs behind \(X\) (it will be proved later that for monotonously increasing \(V(x) > 0\) the derivative \(\frac{dE_n(X)}{dX} \geq 0\) for any \(X\) and \(n\)). The magnitude of the displacement, however, for finite barriers, may rise and fall with growing \(X\), as we will see in subsection 3.6.\footnote{This formula was derived by O. Heinonen and S. Taylor using variational principle, see \cite{2}.} \footnote{This follows from a simple variational argument.}
3 The elementary rectangular step model.

Let us now concentrate on the case of abrupt potentials. The basic potential of this kind is a single rectangular barrier \( V(x) = V\theta(x) \). Generalizations to several steps or to less abrupt barriers will be considered later. We start with an analytic perturbative treatment of small barriers which will be shown to contain all the qualitative features of the exact solutions.

3.1 Approximate calculation.

If \( V \ll \bar{h}\omega_c \) or if a state is not very close to the interface, we can use the perturbation theory around Landau levels to calculate the dispersion relation \( E_n(X) \). The perturbed energies to the first order in the barrier potential \( V \) are:

\[
E_n(X) = (n+1/2)\hbar\omega_c + \left< n, X | V\theta(x) | n, X > \right> + V \int_0^\infty dx \rho^0_n(X, x)
\]

where \( \rho^0_n(X, x) \) is the electron density corresponding to the solution of eq.(3) without the barrier. It is given by

\[
\rho^0_n(X, x) = \rho^{Lan}_n(x - X)
\]

\[
\rho^{Lan}_n(x) \equiv \frac{1}{\sqrt{\pi 2^n n!}} \frac{x}{l^2} e^{-x^2/l^2} H_n^2(x/l)
\]

where \( H_n(x) \) are the Hermite polynomials of the order \( n \). The integral can be performed to obtain analytic expressions for the first order corrections of
the energies:

\[
\Delta E_0 = V \left[ 1/2 + 1/2 \text{Erf}(X/l) \right]
\]

\[
\Delta E_1 = V \left[ 1/2 + 1/2 \text{Erf}(X/l) - \frac{X/l}{2\sqrt{\pi}} \exp \left(-\frac{X^2/l^2}{2}\right) \right]
\]

for the first two levels. Differentiating eq.(7) with respect to \(X\) one obtains:

\[
\frac{\partial E_n(X)}{\partial X} = V \rho_{n}^{\text{Land}}(X).
\]

The inverse density of states of the \(n^{th}\) Landau branch is proportional to \(\frac{\partial E_n(X)}{\partial X}\). Now, since the electron density, eq.(8), has \(n\) nodes, perturbatively, there are precisely \(n\) infinitely flat regions of the dispersion relation. These will be called edge plateaus. For example, \(E_1(X)\) has such region around \(X = 0\). Generally, the zeros of the Hermite polynomials thus determine the plateau centers.

The gap between the ground and the first excited Landau branches does not remain \(\hbar \omega_c\). For \(X > 0\) it gets reduced and reaches its minimum value \(\hbar \omega_c - \frac{e^{-1/2}}{2^{3/2}\sqrt{\pi}} V\) at \(X = l/\sqrt{2}\).

These two features turn out to be of general nature rather than just an artifact of the perturbation theory. As we show next, they become even more pronounced for higher barriers.

### 3.2 Spectrum.

In order to solve the quantum mechanical problem eq.(3) with the rectangular potential for arbitrary height \(V\) beyond perturbation theory, the usual
quantum mechanical matching of the wave function has to be performed along the boundary line \( x = 0 \). This was done for the finite barrier in \([?]\) (in which, however, the edge plateaus have not been noted).

The wave function matching for \( \phi_{n,X}(x) \) has to be performed at a single point \( x = 0 \). It is convenient to shift the origin of the coordinate system to \( X \). In natural units of magnetic length the new variable \( x' \) is: \( x' \equiv \sqrt{2}(x - X) \).

With energy expressed in units of Landau spacing \( \hbar \omega_c \), \( \nu_n \equiv E_{n,X}/(\hbar \omega_c) - \frac{1}{2} \), eq.(3) takes a form

\[
\frac{d^2}{dx'^2} - \frac{1}{4}x'^2 - V\theta(x' + \sqrt{2}X/l) + \left( \nu_n + \frac{1}{2} \right) \phi_{n,X}(x') = 0 \quad (11)
\]

which is the differential equation defining the parabolic cylinder functions \([?, ?]\). The two linearly independent solutions \( D_{\nu_n}(-x') \) and \( D_{\nu_n-V}(x') \) satisfy asymptotically the conditions of rapid decrease for \( x' \to -\infty \) and \( x' \to +\infty \), respectively.

The matching of the logarithmic derivatives at \( X' = -\sqrt{2}X/l \) (or equivalently the condition of zero Wronskian in the expression for the Green’s function of the system) gives:

\[
\frac{D'_{\nu_n-V}(x'|_{x'=X'})}{D_{\nu_n-V}(X')} - \frac{D'_{\nu_n}(-x'|_{x'=-X'})}{D_{\nu_n}(-X')} = 0 \quad (12)
\]

This determines the energy levels \( \nu_n \) as functions of the position \( X \). The equation (12) was solved numerically using a simplified form (obtained from the well known relations expressing derivatives of the parabolic cylinder func-
\[ D_{\nu_{n+1}}(X')D_{\nu_n-V}(-X') + D_{\nu_{n-V+1}}(-X')D_{\nu_n}(X') = 0 \] (13)

The dispersion relations for electrons \( E_n(X) \) (Landau branches) in the vicinity of the barrier have been evaluated numerically. Results for \( V = \hbar \omega_c \) and \( V = 5\hbar \omega_c \) are given in Fig.1 and Fig.2. The ground Landau branch behaves as expected. It starts at its left asymptotic value \( \nu = 0 \) and gradually rises to the right asymptotic value \( V + \nu \). The spectrum of excited Landau branches above the top of the barrier is rather surprising, however. Instead of smooth transition from one asymptotic region \( (X << 0) \) to another \( (X >> 0) \), a steplike rise is obtained. Two unexpected features can be clearly seen:

(i) **Edge plateaus.**

The \( n^{th} \) Landau branch \( E_n(X) \) has \( n \) very pronounced edge plateaus. We call these edge plateaus in order to differentiate them from those in the asymptotic regions (the bulk plateaus). Density of states at the edge plateau energies is strongly enhanced.

(ii) **Landau gap reductions.**

The \( n^{th} \) Landau branch almost touches the \( (n-1)^{th} \) one \( n \) times. Unlike in the case of smooth confinement in which all the Landau branches follow the underlying potential \[ \underline{\; \;} \], the energy gap between two neighbouring branches exhibits regions of significant reduction, in particular for higher barriers.

\[ ^4 \text{Results for a high barrier } V = 5 \hbar \omega_c \text{ were reported earlier \cite{??}.} \]

\[ ^5 \text{Similar behaviour is observed in the opposite extreme case of abrupt and infinite barrier \cite{??}.} \]
Following a Landau branch edge plateaus and the gap reduction regions alternate. First we would like to understand the origin of the edge plateau phenomenon.

3.3 Why there are infinitely flat plateaus for the step potential?

The plateaus in Fig 1 and 2 look, in fact, very flat. How flat? In order to see this, we calculate the density of states $D(E)$. As it is well known [?] the density of states in 1D system is just an inverse of the derivative

$$D_n(E) = \frac{1}{2\pi} \left[ \frac{dE_n(k_y)}{dk_y} \right]^{-1} = \frac{1}{2\pi l^2} \left[ \frac{dE_n(X)}{dX} \right]^{-1}$$

(14)

Fig.3 shows the density of states of the third excited $n = 3$ Landau level for $V = 5\hbar \omega_c$. The three peaks around $\nu = 5.7$, $\nu = 6.4$ and $\nu = 7.1$ indicate infinite density of states. In Fig.4, full density of states from all the branches below Fermi level $E_F = 3.5 \hbar \omega_c$ is plotted.

Now we will show that this is indeed the case for any rectangular potential. We apply the Hellmann - Feynman theorem to Hamiltonian eq.(11), again with respect to $X$, to obtain:

$$\frac{dE_n(X)}{dX} = <\phi_{nX}|V\delta(x + X)|\phi_{nX}> = V|\phi_{nX}(x' = -X)|^2$$

(15)

Returning back to the variable $x$ the result is

$$\frac{dE_n(X)}{dX} = V\phi_{nX}^2(x = 0)$$

(16)
This is the square of the (real) wave function at the interface. Note that from eq. (16) we can obtain the monotonicity of $E_n(X)$\footnote{It is convenient to use eq. (16) to normalize the wave functions. This circumvents the numerical integration.}

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