Boundary Conditions for Bulk and Edge States in Quantum Hall Systems

E. Akkermans, J. E. Avron, R. Narevich
Department of Physics, Technion, 32000 Haifa, Israel
and R. Seiler
Fachbereich Mathematik, TU-Berlin, Germany
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For two dimensional Schrödinger Hamiltonians we formulate boundary conditions that split the Hilbert space according to the chirality of the eigenstates on the boundary. With magnetic fields, and in particular, for Quantum Hall systems, this splitting corresponds to edge and bulk states. Applications to the integer and fractional Hall effect and some open problems are described.

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The theory of the Quantum Hall Effect has been torn between several schools of thought: one stresses the two dimensional bulk aspects of the interior[1]; another emphasizes the importance of the one dimensionality of the edge[2] and other points of view focus on the interplay between bulk and edge[3]. It is therefore remarkable that in spite of this the notion of bulk and edge of a quantum system has not been formulated as a sharp dichotomy even for idealized situations. Classically, there is such a dichotomy for billiards in magnetic fields: orbits that lie in the interior rotate one way, clockwise for positively charge particles, while orbits that hit the edge make a skipping orbit and rotate counter-clockwise[4]. Bulk and edge are therefore distinguished by the chirality relative to the boundary. Our purpose here is to formulate a corresponding dichotomy in quantum mechanics. As we shall explain this can be achieved by imposing certain *chiral* boundary conditions for Schrödinger and Pauli operators.

The chiral boundary condition we introduce is sensitive to the direction of the (tangential) velocity on the boundary. For (separable) quantum billiards this enables us to split the one particle Hilbert space into a direct sum of two orthogonal, *infinite dimensional* spaces with positive and negative chirality on the boundary. In the presence of a magnetic field, this split gives a Hilbert space for edge states, $\mathcal{H}_e$, and a Hilbert space for bulk states, $\mathcal{H}_b$, such that the full Hilbert space is $\mathcal{H} = \mathcal{H}_e \oplus \mathcal{H}_b$. Subsequently we shall explain how chiral boundary conditions are formulated for Schrödinger Hamiltonians which do not necessarily correspond to separable billiards, i.e. Schrödinger Hamiltonians with background potential and electron-electron interactions.

The chiral boundary condition we introduce is a relative of a boundary condition introduced by Atiyah, Patodi and Singer (APS) in their studies of Index theorems for Dirac operators with boundaries[5]. However, the chiral boundary condition we shall introduce differs from it in an important way, as we shall explain below.

The splitting of the Hilbert space comes with a splitting of the quantum billiard Hamiltonian and its spectrum to a bulk piece and an edge piece. As we shall see, it is a property of the chiral boundary conditions that the bulk spectrum has a ground state at precisely the energy of the lowest Landau level in the infinite plane, and a degeneracy which is the total flux through the billiard, (corrected to an integer number of flux units by a boundary term). The bulk energy spectrum has a gap above the ground state, which for separable billiards, is the gap between Landau levels in the infinite plane. Since this gap survives in the thermodynamic limit of a billiard of infinite area, the bulk ground state is guaranteed to be incompressible in this sense.

In contrast, the edge spectrum, in the thermodynamic limit of long boundary is gapless. In this limit, the edge states have a well defined "sound velocity", which reflects the linearity of the dispersion relation at low energies. The sound velocity v is

$$v/c = k\lambda_c \,/\ell_B, \tag{1}$$

where k is a dimensionless (nonuniversal) constant, c is the velocity of light , $\lambda_c = \frac{\hbar}{mc}$ is the Compton wavelength of the electron and $\ell_B = \sqrt{\Phi_0/B}$ is the magnetic length. This sound velocity is very small in all reasonable magnetic fields.

The splitting of the Hilbert space enables us to describe charge transport in terms of spectral flow. In particular, (adiabatic) gauge transformations can transfer states between $\mathcal{H}_e$ and $\mathcal{H}_b$. For the semi-infinite cylinder, such a spectral flow is described below. This generalizes the Index theory of the Integer quantum Hall effect[6] to systems with boundaries.

We start with the semi-infinite cylinder for which we shall illustrate the chiral boundary condition. The Landau Hamiltonian with chiral boundary condition is separable and a complete spectral analysis can be made.

Consider the semi-infinite cylinder, M, in $\mathbb{R}^3$, whose boundary ∂M is a circle with a circumference ℓ: $M = \{(x,y)\,|\; -\infty \le x \le 0,\ 0 \le y < \ell\ \}$. The orientation of M and the orientation of the boundary, ∂M, are linked by requiring that traversing the boundary in the positive direction keeps M on the *left* hand side.

A constant magnetic field perpendicular to the surface, of strength $B > 0$ and with outward orientation acts on the surface. We take the charge of the electron to be positive (sic!) so classical (bulk) electrons in the interior of M rotate clockwise. In addition we assume that a flux tube carrying flux ϕ threads the cylinder. We shall regard ϕ as a parameter, while B is kept fixed throughout. A gauge field describing the situation is $A(\phi) = (0, Bx + \phi/\ell)$. The velocity operator, in units $m = \hbar = e/c = 1$, is $(v_x, v_y) = (-i\partial_x, -i\partial_y - Bx - \phi/\ell)$. The classical energy associated to a particle on a billiard is purely kinetic, $E = v^2/2$. The corresponding quantum Hamiltonian is the Landau Hamiltonian given formally by the second order partial differential operator:

$$2H_L(\phi) = D^\dagger(\phi)D(\phi) + B, \tag{2}$$

where $D(\phi) = iv_x - v_y(\phi, x) = \partial_x + (i\partial_y + Bx + \phi/\ell)$.

For this to define a self-adjoint operator in the one particle Hilbert space we need to specify boundary conditions on ∂M.

The chiral boundary condition that we introduce requires different things from the wave function on the boundary depending on the tangential velocity, $v_y(\phi, x)$ at the boundary $x = 0$. Since $v_y(\phi, 0) = -i\partial_y - \phi/\ell$ commutes with D we separate variables, and describe the chiral boundary conditions for the resulting ordinary differential operators on the half line $-\infty \le x \le 0$, parameterized by $m \in \mathbb{Z}$ and $\phi \in \mathbb{R}$:

$$2H_m(\phi) = -\frac{d^2}{dx^2} + \left(\frac{2\pi m - \phi}{\ell} - Bx\right)^2. \tag{3}$$

Let

$$D_m(\phi) = \frac{d}{dx} - \frac{2\pi m - \phi}{\ell} + Bx. \tag{4}$$

The chiral boundary condition requires:

$$\begin{aligned} D_m f_m\Big|_{x=0} &= 0, \ \text{if} \ v_y(\phi,0) = \frac{2\pi m \ - \phi}{\ell} \le 0; \\ (iv_x)\, f_m\Big|_{x=0} &= 0, \ \text{if} \ v_y(\phi,0) = \frac{2\pi m \ - \phi}{\ell} > 0. \end{aligned} \tag{5}$$

Recall that a classical electron in the bulk rotate clockwise, and so its velocity near the boundary *disagrees* with the orientation of the boundary. For such an electron we require *spectral* boundary conditions, $(D_m f)(0) = 0$, which are m-dependent elastic boundary conditions (an interpolation between Neumann and Dirichlet). A classical skipping orbit near the boundary moves in a direction that agrees with the orientation of the boundary, and for positive velocity on the boundary we impose Neumann boundary condition. We shall say more on the reasons for choosing spectral and Neumann for the different chiralities below.

Since both the differential operator, and the boundary conditions are defined in terms of the velocity, gauge invariance is manifest. Moreover, it can be checked that the boundary conditions in Eq. (5) define a self-adjoint eigenvalue problem, which we shall call the chiral Landau Hamiltonian. The spectrum and eigenfunctions can be described in terms of special functions[7].

FIG. 1. Spectrum of the Landau Hamiltonian.(a) with chiral (solid lines) and Dirichlet (dashed lines) boundary conditions (inset- enlarged box, showing a cusp between bulk and edge states), (b) with APS boundary conditions.

The bulk space $\mathcal{H}_b$ is defined by

$$\mathcal{H}_b = \bigoplus_{2\pi m \le \phi} e^{2\pi i m y/\ell} f_m(x), \tag{6}$$

where f_m are the eigenfunctions of the chiral Landau Hamiltonian that satisfy spectral boundary condition. $\mathcal{H}_e$, the space of edge states, is the orthogonal complement. The spectrum for the chiral Landau Hamiltonian is shown in Fig. 1.a as a collection of curves plotted as functions of the velocity on the boundary. The bulk spectrum is determined by the left part of the figure i.e. by negative values of the velocity and the edge spectrum by the right part (positive values). The ground state of the bulk spectrum has energy $B/2$ which corresponds to the lowest Landau level in the plane (doubly infinite cylinder). Like it, it is infinitely degenerate. This turns out to be a property of chiral boundary conditions that holds for a large class of billiards: the ground state of the bulk spectrum has energy $B/2$ and the degeneracy is (an integer close to) the total flux through the billiard. The present case where the total flux is infinite is an example. The bulk ground state is separated by a gap B from the first excited bulk state. For the excited bulk states the situation is more complicated, and one general statement is that the essential bulk spectrum, coincides with the spectrum of the Landau Hamiltonian in the plane: that is, the bulk spectrum differs from the Landau spectrum by at most a discrete set of eigenvalues.

The edge spectrum, in contrast, is, for any finite boundary length ℓ, purely discrete (the essential spectrum is empty). In the thermodynamic limit $\ell \to \infty$ the edge spectrum becomes gapless. The slope of the curves describing the edge spectrum give a linear dispersion with a finite sound velocity as $v_y(\phi, 0) \searrow 0$. In particular, for the lowest edge branch one has, in the limit $\ell \to \infty$, a unique sound velocity for the chiral edge currents:

$$\left.\frac{\partial E_0}{\partial v_y}\right|_0 = \sqrt{\frac{B}{\pi}} \tag{7}$$

This fixes the k in Eq. (1) in this case. It is worth emphasizing the existence of the cusp between bulk states and the corresponding edge branch as shown in Fig.1.a.

It is instructive to compare the spectral properties of the Chiral Landau Hamiltonian with the Dirichlet Landau model, where one replaces Eq. (5) by the requirement $f_m(0) = 0$ for all m. This too can be solved explicitly in terms of special functions[7] and the spectrum is shown in Fig. 1.a. The corresponding curves unlike the chiral case are analytic functions. This has some immediate implications: First, there is no sharp line of divide between edge and bulk, second, there is no natural sound velocity because the dispersion law is not linear at small energies, and finally, there is no macroscopic degeneracy of the ground state (or any other state).

The chiral boundary condition Eq. (5) is a close relative of boundary conditions introduced in [4]. APS boundary condition replaces Eq. (5) by

$$\left(\frac{d}{dx} - \frac{2\pi m - \phi}{\ell}\right) f_m\Big|_{x=0} = 0 \quad \text{if } v_y(\phi,0) \le 0;$$
$$f_m\Big|_{x=0} = 0 \quad \text{if } \ v_y(\phi,0) > 0. \tag{8}$$

That is, the Neumann piece for the edge states is replaced by Dirichlet. Here too there is a sharp divide of the states according to their chirality. But, in APS the putative edge states with the good chirality are forced to have vanishing density near the boundary and tend to be pushed away from the edge. These can not be bona fide edge states. The APS Landau Hamiltonian can be solved explicitly for the problem at hand, and the spectrum is shown in Fig. 1.b. The glaring difference with Fig.1.a is that now the energy curves are *discontinuous*. As we shall explain, this discontinuity has undesirable features for studying spectral flows and transport in quantum mechanics.

Consider now the spectral flow resulting from the increase of the threading flux ϕ by a unit of quantum flux: $\phi \to \phi + 2\pi$. By inspection of Fig.1 one sees that all states in the diagrams move one notch to the left. In the chiral and APS cases which have a clear divide between chiralities we see that each branch of the good chirality looses a state and each branch of the bad chirality gains one. In the chiral case (Fig.1.a) one can follow continuously each state as its chirality changes. In Fig.1.b this is not the case. Chiral boundary conditions therefore give a way of counting the charge being transport from bulk to edge. The same spectral flow takes place for the Dirichlet spectrum except that here what is edge and what is bulk is a vague notion which does not allow for counting the states that move from edge to bulk. In the case of APS the notion of edge and bulk is sharp, but because of the discontinuity of the curves in Fig.1.b there is no way to identify the flow of bulk to edge.

It is also instructive to examine how chiral boundary conditions are related to Laughlin states. As we shall see, Laughlin states for filling fraction $1/M$, M an odd integer, are bulk states with maximal density.

To simplify the notation let us take a cylinder of area 2π, $M = \{(x,y) \mid \ -1 \le x \le 0,\ 0 \le y < 2\pi\ \}$. We shall take $\phi = 0$ in what follows. The Laughlin state of the (doubly infinite) cylinder for filling fraction $1/M$, with M odd is[9]

$$\psi_L = \prod_{1\le j<k\le N} \left(e^{-z_j} - e^{-z_k}\right)^M \prod_{1\le k\le N} e^{-Bx_k^2/2 + mz_k}. \tag{9}$$

Here $z = x + iy$ and $m \in \mathbb{Z}$. Fix a particle, say $z = z_1$. As a function of z, ψ_L has the form

$$\left(A_1 e^{-M(N-1)z} + A_2 e^{-M(N-2)z} + \dots\right) e^{-Bx^2/2 + mz} \tag{10}$$

where A_j are independent of z. The chiral boundary conditions for z need to be imposed on the two bounding circles at $x = 0$ and $x = -1$ with opposite orientations. Since ψ_L is in the kernel of D, $(D\psi_L = 0)$, the spectral boundary conditions are automatically satisfied. So, all that needs to be checked is that the velocity on the two bounding circles is anti-chiral. That is:

$$m + B \ge M(N-j) \ge m, \tag{11}$$

for all $1 \le j \le N$. $j = N$ sets $m = 0$, and $j = 1$ sets an upper bound on the number of electron that the Laughlin state may accommodate and still satisfy the chiral boundary conditions : $N \le 1 + B/M$. Recall that the area of the cylinder is 2π, so that B is the total flux in units of quantum flux. In the (thermodynamic) limit of large flux the maximal filling is $N/B \to 1/M$, which is what Laughlin plasma argument gives[8].

The case of other separable billiards, such as a circular disc can be treated in a similar way. The new feature that arises for separable billiard of finite area is that there are interesting index theorems for the degeneracy of the chiral bulk ground state. These issues will be described elsewhere[10].

We now turn to the description of the chiral boundary conditions for more general Schrödinger operators and give further motivation for them. It turns out that once chiral boundary conditions have been formulated for the non separable case further generalization to Schrödinger operators with background potential and to multielectron systems where electrons are allowed to interact, follow. For the sake of simplicity and concreteness we shall stick to one electron billiards. Moreover, to avoid writing complicated formulas, we shall assume that the two dimensional manifold M is (metrically) cylindrical near its boundary ∂M.

It is instructive to formulate the chiral boundary conditions in terms of quadratic forms, and to compare them with the classical boundary conditions, Dirichlet and Neumann. A positive quadratic form, $Q(\varphi)$, on a dense domain, uniquely defines a self-adjoint operator[11]. The nice thing about quadratic forms is that the boundary conditions are part of the form and suggest a physical interpretation. Let $\langle\cdot|\cdot\rangle_M$ stands for the scalar product in

$L^2(M)$ and $\langle\cdot|\cdot\rangle_{\partial M}$ for the scalar product on the boundary of M. $C^\infty(M)$ is the space of smooth functions on M. The quadratic form

$$Q(\varphi) = \langle\nabla\varphi|\nabla\varphi\rangle_M + \lambda\,\langle\varphi|\varphi\rangle_{\partial M} \tag{12}$$

with $\varphi \in C^\infty(M)$ and $0 \le \lambda < \infty$, describes for $\lambda = 0$ the Neumann problem and for $\lambda \to \infty$ the Dirichlet problem for the Laplacian Δ. For finite λ one has the elastic boundary conditions. The Neumann problem says that the boundary term gives no penalty (in energy) if there is density on the boundary, while, Dirichlet says that the penalty is large and so finite energies have zero density on the boundary. It is an immediate consequence of the quadratic form and the variational principle that the Dirichlet spectrum have energies above the Neumann spectrum. λ scales like the inverse of a length squared so that in the absence of a dimensional parameter, Dirichlet and Neumann are distinguished.

Dirichlet and Neumann associate a penalty for density at the boundary. Chiral boundary conditions associate a penalty for a chirality. Since we want edge states (which have positive chirality) to pay a price and bulk states (which have negative chirality) not to affected by the boundary, a quadratic form which does that in the presence of gauge fields is:

$$\begin{aligned} Q_c(\varphi) &= \langle D\varphi|D\varphi\rangle_M + \lambda\Big\langle\varphi\Big|v_+\varphi\Big\rangle_{\partial M} \\ v_+ &= \begin{cases} v_y & if\ v_y > 0; \\ 0 & otherwise, \end{cases} \end{aligned} \tag{13}$$

where $\varphi \in C^\infty(M)$, $0 \le \lambda < \infty$ and v_y is the operator of (tangential) velocity on the boundary. Now, in contrast to the Dirichlet-Neumann case discussed above, λ is dimensionless. To see what this implies for the boundary conditions we need to go to the operator and its domain. The domain of $D^\dagger D$ consists of all smooth functions, such that

$$\langle D\varphi|D\cdot\rangle_M + \lambda\Big\langle\varphi\Big|v_+\cdot\Big\rangle_{\partial M}, \tag{14}$$

is a L^2–bounded linear functional. Integration by parts in the variable x leads to

$$\langle D^\dagger D\varphi|\cdot\rangle_M + \Big\langle(D+\lambda v_+)\varphi\Big|\cdot\Big\rangle_{\partial M}. \tag{15}$$

For this to define a linear functional, the term on the boundary must vanish identically for all φ in the domain of $D^\dagger D$. If we write $\varphi = \varphi_+ + \varphi_-$, where φ_+ restricted to ∂M belongs to the positive spectral subspace of v_y this gives: $D(H_L) = \Big\{\varphi|\ \varphi \in C^\infty(M)\,, \Big(d_x + (\lambda-1)v_y\Big)\varphi_+ = 0\,, D\varphi_- = 0\Big\}$. $\lambda = 0$ gives spectral boundary condition for both chiralities. $\lambda = 1$ gives spectral boundary conditions for negative chiralities and Neumann for positive chiralities. In the separable case this gives the chiral boundary conditions Eq. (13). $\lambda = \infty$ gives the APS boundary conditions. In principle, one could take λ as a parameter in the theory, fixed by the sound velocity for the edge states. $\lambda = 1$ is distinguished in tending to maximize the density of the edge states at the boundary.

The quadratic form is gauge invariant and non-negative and therefore defines a non-negative, gauge invariant, Hamiltonian associated to kinetic energy: $H_L = D^\dagger D \ge 0$. The Hamiltonian H_L is symetric by a direct calculation.

Chiral Schrödinger Hamiltonians define a self-adjoint eigenvalue problem. This is true irrespective of whether the problem is separable or not; if there is a background scalar potential or not, and even if one considers a one electron theory or a multielectron Hamiltonian. However, only in the separable one particle case, (and slightly more general but still nongeneric cases), does one have a clean splitting of the eigenspaces of the Hamiltonian into two pieces: $\mathcal{H}_e$ and $\mathcal{H}_b$. In general, an eigenstate φ will have both a non-zero φ_+ and φ_- piece, and the spectral subspaces do not split cleanly. The best one might expect in the non separable case is that in certain limits eigenstates will have a dichotomy. Namely, either φ_- or φ_+ will be small in the limit for every eigenstate. Examination of simple examples suggests that in the limit of large magnetic fields, $B \to \infty$, there is such an asymptotic splitting. Similarly, it would be interesting to formulate a corresponding splitting principle in the multiparticle Fock space. Both questions are open and interesting.

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