PHILOSOPHICAL MAGAZINE B, 1998, VOL. 77, NO. 5, 1097–1105

Chiral boundary conditions for quantum Hall systems

By E. AKKERMANS and R. NAREVICH
Department of Physics, Technion, Haifa, 32000, Israel

ABSTRACT
A quantum mesoscopic billiard can be viewed as a bounded electronic system due to some external confining potential. Because, in general, we do not have access to the exact expression of this potential, it is usually replaced by a set of boundary conditions. We discuss, in addition to the standard Dirichlet choice, the other possibilities of boundary conditions which might correspond to more complicated physical situations including the effects of many-body interactions or of a strong magnetic field. The latter case is examined more in details using a new kind of chiral boundary conditions for which it is shown that, in the quantum Hall regime, bulk and edge characteristics can be described in a unified way.

§ 1. INTRODUCTION

One of the main issues in quantum mesoscopic physics is to study the behaviour of many-particle quantum systems in confined geometries. For many purposes the many-body interactions are negligible and the problem reduces to those of one particle in a confined geometry. The corresponding Hamiltonian is a sum of a kinetic term and a one-body operator describing either the confining potential or the disorder in the bulk of the system. The expression 'quantum mesoscopic billiards' (QMBs) was coined to describe generically this class of problems. The role played by the boundaries in the behaviour of QMBs is central. In the absence of bulk disorder, the shape of the boundary determines the nature of the energy spectrum, that is whether or not the system will show quantum signatures of chaos.

The aim of this article is twofold. First, it is to discuss in general terms what motivates the choice of a given set of boundary conditions and to see under which conditions this choice is justified for confined quantum systems in situations other than the QMBs defined above, for instance for a many-body system when the Hamiltonian is no longer quadratic or in the presence of a high magnetic field, that is in the quantum Hall regime.

§ 2. HOW TO CHOOSE BOUNDARY CONDITIONS?

Consider the case of a QMB without bulk disorder. It is described by the Hamiltonian $H = -(\hbar^2/2m)\Delta + V(r)$, where $V(r)$ is a confining potential. It is built up microscopically from the electrostatic description of two electron gases of different dielectric characteristics. For a given ratio of the dielectric constants, the effective image force is strong enough to keep the electrons localized in a given area (the billiard). To know exactly the shape of the potential $V(r)$ and to solve for it the Schrödinger equation is a hopeless task. Then, under the assumption that $V(r)$ has bound states, it is possible to replace this problem by a simpler problem, supposedly equivalent, defined by $H = -(\hbar^2/2m)\Delta$ and $\psi|_{\mathcal{B}} = 0$ for the wavefunction, where the boundary $\mathcal{B}$ is obtained from the symmetry and the shape of $V(r)$. This is the so-called Dirichlet choice and it is widely used to describe QMBs. A more technical remark is perhaps appropriate at this stage. This kind of 'box quantization' obtained using Dirichlet boundary conditions is also widely used to describe other physical situations, for instance transport in a quantum system. Here, unlike the QMB case, the coupling to the external world through 'leads' plays a central role and the spectrum of the whole system is continuous. This leads very often to ill defined or diverging quantities which are regularized using instead a discrete spectrum. To this aim, the Dirichlet choice is also used among others, assuming that it describes hopefully the same physics in the limit when the boundary recedes to infinity. I shall not discuss this issue any further (Akkermans 1997).

Although the Dirichlet choice is the most popular for the reasons discussed above, it is not the only one and may even lead to unpleasant surprises. Consider for instance the case of a confined Dirac particle (a Dirac billiard) described by

$$\begin{bmatrix} 0 & D^{\dagger} \\ D & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = E \begin{bmatrix} u \\ v \end{bmatrix}$$

instead of a Schrödinger Hamiltonian. Here, D and $D^{\dagger}$ are first-order differential operators (the roots of the Laplacian) and the wavefunction $\psi = \left[\begin{smallmatrix} u \\ v \end{smallmatrix}\right]$ is a two-component spinor. By demanding Dirichlet boundary conditions, the problem is overdetermined and ψ is identically zero not only on the boundary but also in the whole system. It is also known for this problem that other choices of local boundary conditions (e.g. Neumann conditions) lead to difficulties associated with the creation of particle–hole pairs (the Klein paradox) (Berry and Mondragon 1987). This problem is not only an academic curiosity, but also might be relevant if one wants to describe mesoscopic superconducting billiards where the spectrum is obtained from the Bogoliubov–deGennes Hamiltonian which, when linearized, belongs to the class of Dirac problems.

§ 3. Beyond one particle: effective Hamiltonians

So far we have considered the case of quadratic Hamiltonians, that is the Laplacian plus a (one-body) confining potential. When many-body effects cannot be neglected any longer, the situation is far more complicated. A standard form for the (tight-binding) Hamiltonian is

$$H = \sum_i \epsilon_i c_i^{\dagger} c_i + \tfrac{1}{2} \sum_{ijkl} \langle ik|V|jl\rangle c_i^{\dagger} c_k^{\dagger} c_l c_j .$$

The kinetic part is still given (in a second quantized form) by a sum of Laplacian operators, but the second part associated with the interaction is a quartic term. Except for some special cases, we do not know how to diagonalize such Hamiltonians no matter whether the system is bounded or not. The main issue underlying the search of various approximations is precisely to define instead an effective quadratic Hamiltonian whose parameters depend on the approximation. The well known perturbative or variational methods (Hartree–Fock, random-phase approximation (RPA), Bogoliubov, etc.) do fulfil this objective. When dealing with confined many-body systems, we need to build an effective quadratic Hamiltonian whose potential takes into account both the many-body effects of the confined electrons but also, just like before, the effects of the electrostatic potentials resulting from the interactions with the surrounding environment.

Our choice of boundary conditions for the effective one-body (quadratic) Hamiltonian is now broader and depends on the nature of the confining potential. If it is due to image forces as for the QMB case, then the Dirichlet choice will again be justified, but, if the confinement is dominated by the many-body effects in the system itself, then we might be led to other choices of boundary conditions.

For the benefit of the more pragmatically inclined reader, let us illustrate these ideas by the example of the Feynman *Ansatz* for N strongly interacting bosons (Feynman 1954). The many-body Hamiltonian is

$$H = E_0 - \frac{\hbar^2}{2m}\sum_i \Delta_i + V,$$

where $V = \sum_{ij} V(|r_i - r_j|)$ is the interaction potential and E_0 the ground-state energy. The N boson wavefunctions describing the excited states are assumed (Feynman *Ansatz*) to be of the form $\Psi(r_1, \ldots, r_N) = F\Psi_0(r_1, \ldots, r_N)$, where $F = \sum_i^N f(r_i)$ and Ψ_0 is the exact (but unknown) ground-state wavefunction. This form is exact for the non-interacting case, but it assumes for the interacting case that the interactions build up separately (under an adiabatic switching) in F and in Ψ_0. This approximation may be shown to be equivalent (under certain conditions) to the RPA, the generator coordinate method (Jancovici and Shiff 1964) or the quasiboson approximation. The equation of motion of the complex function $f(r)$ (it is not the wavefunction) is obtained by minimizing the energy $E = \langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$. Under the assumption of an incompressible ground state of density ρ_0, $\delta E = 0$ implies that

$$-\frac{\hbar^2}{2m}\rho_0\nabla^2 f = E\int \mathrm{d}\mathbf{r}' f(\mathbf{r}')\rho(\mathbf{r}-\mathbf{r}'),$$

where $\rho(\mathbf{r}-\mathbf{r}')$ is the density correlation function in the ground state Ψ_0. The effective energy E is now given by the quadratic form

$$E = -\rho_0\frac{\hbar^2}{2m}\int \mathrm{d}\mathbf{r}\, f^*\nabla^2 f$$

and, to obtain the spectrum, we have to impose boundary conditions on the function f. Assuming translational invariance, Feynman obtained the well known relation $E = (\hbar^2/2m)[k^2/S(k)]$, where $S(k)$ is the structure factor. This gives the one-branch phonon spectrum for small k. For a bounded system, relating $f(r)$ to the order parameter, we obtain that the fluid velocity is $\mathbf{v}(r) = (1/m)\nabla f$ so that the natural boundary conditions are of Neumann type, $\hat{\mathbf{n}}\cdot\nabla f|_B = 0$, where $\hat{\mathbf{n}}$ is a unit vector normal to the boundary. The same kind of approach applies to the case of bounded superconductors where the natural boundary conditions for the effective quadratic Hamiltonian are now generalized (deGennes 1966) to

$$\hat{\mathbf{n}}\cdot\left(-\mathrm{i}\hbar\nabla - \frac{2e}{c}\mathbf{A}\right)\Big|_B = \mathrm{i}\lambda f,$$

where λ is finite for the boundary between a superconductor and a normal metal while it is zero for an insulator.

To conclude, it looks to be quite a general result that, where the Dirichlet boundary conditions are more appropriate for the case of a QMB (i.e. usual quantum mechanics), the Neumann (or elastic) boundary conditions appear to be the natural choice for collective (bosonic) excitations (phonons, plasmons, etc.) which do appear in the effective quadratic approximations of many-body Hamiltonians. This is intimately related to the semiclassical nature of these approximations. They enable us, starting with the microscopic description, to reduce the problem to the study of large-scale modes for which boundary conditions should be formulated, according to macroscopic principles (such as continuity of the current). This leads usually to Neumann boundary conditions.

§4. Bounded quantum Hall systems

The remaining part of this article is devoted to the application of the previous general remarks to the specific case of bounded electrons in a strong magnetic field that is in the quantum Hall regime. We shall focus on the simpler case of non-interacting electrons.

The various descriptions of the quantum Hall effects developed so far belong to two main categories. One is based on a bulk description, that is on the properties of a Landau-like spectrum whose main characteristics are the large degeneracy of the ground state (proportional to the surface of the system) and its incompressibility, that is the existence of a gap between it and the first excited state. These conditions are enough to observe the quantization of the Hall conductance (MacDonald 1995). The surprising stability of these properties with respect to both disorder and interactions are partly responsible for the richness of this problem. Various points of view were developed in order to prove the quantization of the Hall conductance and among them a successful and promising topological approach (Thouless *et al.* 1982, Avron *et al.* 1983). There, using periodic boundary conditions, the system has the topology of a torus so that edge physics does not play any role.

A second line of thought emphasizes the central role played by the edges. It is based on the idea that a magnetic-field-dependent incompressibility always leads to gapless edge excitations. Then, the total current being zero in the bulk (but not the current density), the currents in a Hall experiment flow along the edges (Büttiker 1988, MacDonald 1995).

More recently, these edge states were presented as a possible realization of a quasi-one-dimensional chiral electron gas. Various phenomenological models were developed to describe it, including a chiral Luttinger liquid (Wen 1990, Stone 1991). A global description which would relate these two approaches would be welcome. A microscopic way based on first principles to handle this question is difficult. To know the exact spectrum of the system, we first need to solve a classical electrodynamic problem to obtain the confining potential between two electron gases of different dielectric functions in a strong and inhomogeneous magnetic field. In the absence of applied magnetic field, the bulk excitations are plasmons with a dispersion $\omega \propto k^{1/2}$. In the presence of the magnetic field the bulk spectrum acquires a gap (Kohn's theorem) equal to the cyclotron frequency and chiral edge magnetoplasmons propagating along the boundary do appear with a linear dispersion. Various descriptions were proposed to study these edge excitations using different density profiles (Volkov and Mikhailov 1988, Aleiner and Glazman 1994). Although these approaches do provide a qualitative description of the experimental results (Ernst *et al.* 1996), they do not take into account quantum effects related to the quantization of the Hall conductance, a point which seems to be important experimentally (Ernst *et al.* 1996).

It would be interesting to know whether the microscopic confining potential could be replaced by an appropriate choice of boundary conditions which contain the same physics. To go further, we first consider the case of an effective one-particle Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\left(\nabla - \frac{ie}{\hbar c}\mathbf{A}\right)^2 + V(r,\, B),$$

where $\mathbf{B} = \nabla \times \mathbf{A}$ is the inhomogeneous magnetic field and $V(r, B)$ the effective confining potential, solution of the microscopic electrodynamic problem. To replace $V(r, B)$ by a set of boundary conditions, we have two main possibilities. The first is to assume that it results from the electrostatics interactions and depends very little on the external magnetic field. This situation is similar to the QMBs that we discussed earlier and therefore we shall choose Dirichlet boundary conditions $\psi|_{\mathcal{B}} = 0$. If, on the other hand, the confining nature of the magnetic field plays a role, which is expected at high magnetic fields, then the Dirichlet choice might be incorrect in the sense that, although it confines the electrons, it will not be able to reproduce the edge excitations.

We are therefore looking for boundary conditions which connect together the bulk and edge properties of a confined quantum Hall system. In other words, is there for this problem a generalized Poisson principle for which, like in electrostatics, the bulk and edge excitations are a consequence of one another?

4.1. *Effective boundary conditions*

To go further, we consider the problem of an electron moving in a magnetic field $\mathbf{B}(r) = B\Theta(r - R)\hat{\mathbf{z}}$, that is uniform in a disc of radius R and vanishing outside. The Hamiltonian can then be written

$$\frac{2m}{\hbar^2}H = DD^\dagger - b = D^\dagger D + b,$$

where $D = \exp(\mathrm{i}\theta)\,[\partial_r + (i/r)\partial_\theta + br/2]$ and $b = (eB/\hbar c = 1/l_c^2)$ (l_c is the magnetic length).

4.1.1. *The Dirichlet choice*

Demanding $\psi(R, \theta) = 0$ for the wavefunction, we obtain the spectrum in figure 1, as a function of the angular momentum $m \in \mathbb{Z}$. The main characteristics of this

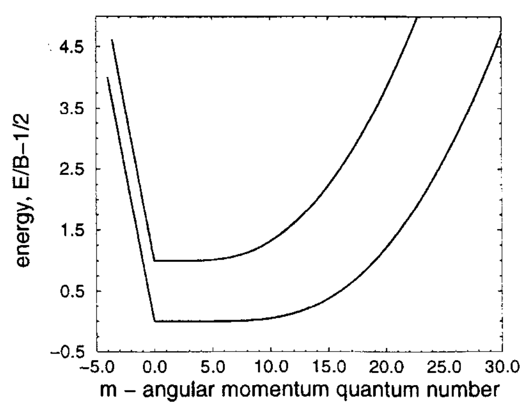

Figure 1. Spectrum of an electron in the magnetic field: Dirichlet boundary conditions.

spectrum are the following.

(1) The lowest Landau level is always below the ground state ($m = 0$), although exponentially close.
(2) For any finite R, the ground state is non-degenerate.
(3) The bulk currents $I = \sum_{m \leqslant m_c} (\partial E_m/\partial m)$, where m_c corresponds to the Fermi energy, are finite and even large.
(4) Since E_m, are analytic functions of m (described as a continuous variable), there is no natural splitting in this spectrum between bulk and edge states.

4.1.2. *The chiral boundary conditions*

One of the main issues concerning the Dirichlet boundary conditions is that they do not provide a sharp dichotomy between bulk and edge states even for idealized situations. It is on the other hand a noticeable fact that such a dichotomy naturally exists for a classical bounded system in a magnetic field; for a given direction of the field, orbits that lie in the interior of the billiard rotate one way, while those hitting the edge make a skipping orbit and rotate in the opposite direction. Bulk and edge states are thus distinguished by their chirality relative to the boundary. Recently, we proposed an extension of such a dichotomy to the quantum-mechanical case (Akkermans *et al.* 1996). Consider for that purpose the tangential velocity operator in the m sector given by $v_m = -m/r + br/2$ with $m \in \mathbb{Z}$ and consider its spectrum $v_m(R)$ projected on the boundary $r = R$. The eigenvalues are given by $v_m(R) = -(1/R)(m - \phi)$, where $\phi = \Phi/\Phi_0$ is the total magnetic flux through the disc in units of the flux quantum $\Phi_0 = hc/e$. The chiral boundary conditions require that

$$\begin{aligned} D_m\psi_m(r)|_{r=R} = 0, \quad \text{if} \quad v_m(R) = -\frac{1}{R}(m-\phi) > 0, \\ \partial_r\psi_m(r)|_{r=R} = 0, \quad \text{if} \quad v_m(R) = -\frac{1}{R}(m-\phi) \leqslant 0, \end{aligned} \tag{1}$$

where $D_m = \partial_r + v_m$. The first condition, as a generalization of the classical case will correspond to a bulk electron for which we demand elastic boundary conditions ($D_m\psi_m(R) = 0$), while the second condition will describe an edge electron for which we demand Neumann boundary conditions. These non-local (spectral) boundary conditions are relatives of the boundary conditions introduced by Atiyah *et al.* (1973) in their study of index theorems for Dirac operators with boundaries precisely for the reasons we discussed earlier. However, they did choose for edge states Dirichlet instead of Neumann boundary conditions here considered for a reason that we shall discuss later. It can be checked directly that this choice preserves gauge invariance and defines a self-adjoint eigenvalue problem. The energy spectrum can be described in terms of special functions and is shown in figure 2. The Hilbert space $\mathcal{H}$ it defines is the direct sum of two orthogonal infinite-dimensional spaces $\mathcal{H}_b$ and $\mathcal{H}_e$ corresponding respectively to bulk and edge states. In contrast with the Dirichlet case, the ground state of the bulk spectrum corresponds precisely to the lowest Landau level and has a degeneracy given by the integer part $[\phi]$ of the total magnetic flux through the disc. The first excited bulk state is separated from the ground state by a gap equal to the cyclotron frequency which ensures incompressibility. Finally, the total current in the ground state is $I = \sum_{m \leqslant [\phi]} (\partial E_m/\partial m) = 0$, a property of the lowest Landau level.

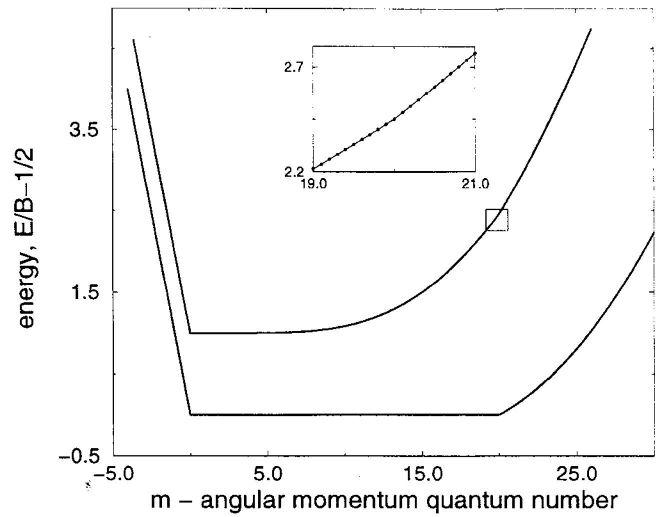

Figure 2. Spectrum of an electron in the magnetic field: chiral boundary conditions. (Inset is an enlargement of the rectangle, showing a cusp between bulk and edge states.)

The edge spectrum is, in contrast, gapless in the thermodynamic limit and has a linear dispersion for low excitation energies with a 'sound velocity' proportional to $B^{1/2}$. The justification of Neumann boundary conditions for the edge states instead of the Dirichlet original choice of Atiyah *et al.* comes from the requirement of having continuous energy curves between bulk and edge energies. Moreover, with the Dirichlet choice, our edge states would have been pushed away from the edge.

4.2. *Spectral flow*

Another interesting difference which does appear in our chiral boundary conditions is the discontinuity in the first derivative of the energy curves. Since this derivative is proportional to the current, such a discontinuity would correspond to a non conservation of the electric charge. Consider now adding an additional time-dependent Aharonov–Bohm magnetic flux at the centre of the disc which may fulfil the role of a battery (electromotive force). Then, by changing it by one unit of quantum flux, one state moves from the bulk to the edge Hilbert spaces. Then, our boundary conditions allow for counting the states that move from bulk to edge. A similar spectral flow takes also place in the Dirichlet case but only in a qualitative sense. Here, we can relate this charge transport (the Hall conductance) to a topological index which characterizes the spectral flow (Akkermans and Narevich 1997).

4.3. *A chiral Hamiltonian for the edge states*

The phenomenological description of the chiral edge states is based on the observation that, as the bulk of the Hall liquid is incompressible and irrotational below the Kohn gap, the only low-energy excitations are on the boundary and may be represented by chiral bosons derived from a Kac Moody algebra (Wen 1990, Stone 1991). The corresponding Hamiltonian can be derived, but a central problem is then to relate it to the bulk quantities. Using our boundary conditions, this bulk-edge relation naturally comes in. Consider the field operators $\hat{\Psi}(r) = \sum_{m=0}^{\infty} a_m \psi_m(r)$, where $\psi_m(r)$ are the eigenfunctions of the one-particle Hamiltonian and a_m the annihilation operator of a state of angular momentum m. Then, up to a constant, the total Hamiltonian can be written in a second quantized form as

$$H = \sum_{m=0}^{\infty} a_m^{\dagger} a_m \int \mathrm{d}^2 r \, \psi_m^*(r) D \, D^{\dagger} \psi_m(r).$$

Integrating by parts, we obtain

$$H = \sum_{m=0}^{\infty} a_m^{\dagger} a_m \left(- \int_{\mathcal{D}} \mathrm{d}^2 r [D\psi_m(r)]^* [D\psi_m(r)] + \int_{\partial\mathcal{D}} \mathrm{d}\theta \, \psi_m^*(R, \theta) \hat{v}(R, \theta) \psi_m(R, \theta) \right)$$

where the first integral is on the disc, while the second is on the circle boundary. These two integrals in the large parentheses define the energy E_m. The ground state corresponds to the full lowest bulk state, that is for angular momentum up to $m = [\phi]$. The lowest excited states are obtained in the limit where m approaches $[\phi]$ from above. In that limit, $D\psi_m(r) = 0$ and only the second integral remains in the Hamiltonian which can be rewritten using the definition of the tangential velocity operator written above:

$$H_{\text{edge}} = -\mathrm{i} \int_{\partial\mathcal{D}} \mathrm{d}\theta \hat{\Psi}^{\dagger}(R, \theta)(\partial_\theta + \mathrm{i}\phi) \hat{\Psi}(R, \theta),$$

which is the Dirac Hamiltonian density for a one-dimensional chiral fermion field whose eigenstates are bosonic excitations.

§ 5. Conclusions

We first notice that, as pointed out before, the bosonic nature of the edge excitations (of linear dispersion) is intimately connected with the choice of Neumann boundary conditions for these states.

Then, the question arises of the generalization of this approach to include interactions (the fractional Hall case) and disorder. Considering the first point, it was shown (Akkermans *et al.* 1996) that, assuming the Laughlin wavefunction for the ground state, and a filling fraction $1/M$ (M being an odd integer), the chiral boundary conditions give precisely the number of states that the Laughlin state as a bulk state can accommodate, that is $N/BR^2 = 1/M$.

For non-separable problems, that is including either bulk disorder or different shapes, it is still possible to use chiral boundary conditions and to obtain a splitting of the Hilbert space. In general, the splitting of the wavefunctions disappears and the states will have instead non-zero parts both in $\mathcal{H}_\mathrm{b}$ and in $\mathcal{H}_\mathrm{e}$.

This approach using non-local boundary conditions might be a promising way to investigate other not unrelated problems such as a rotating superfluid where the Coriolis force is analogous to the Lorentz force in a magnetic field or the Bogoliubov–deGennes equations for a superconducting billiard.

Acknowledgements

It is a pleasure to acknowledge fruitful and numerous discussions with J. E. Avron. This work was supported in part by a grant from the Israel Academy of Sciences and by the fund for promotion of Research at the Technion.

References

Akkermans, E., 1997, *J. math. Phys.*, **38**, 1781.

Akkermans, E., Avron, J. E., Narevich, R., and Seiler, R., 1996, Preprint Cond-Mat/9612063.

Akkermans, E., and Narevich, R.,1997, (in preparation).

Aleiner, I. L., and Glazman, L. I., 1994, *Phys. Rev. Lett.*, **72**, 2935.

Atiyah, M. F., Patodi, V. K., and Singer, I. M., 1973, *Proc. Camb. phil. Soc. math. phys. Sci.*, **77**, 43.

Avron, J. E., Seiler, R., and Simon, B., 1983, *Phys. Rev. Lett.*, **51**, 51.

Berry, M. V., and Mondragon, R. J., 1987, *Proc. R. Soc.* A, **412**, 53.

Büttiker, M., 1988, *Phys. Rev.*, **38**, 9375.

deGennes, P. G., 1966, *Superconductivity of Metals and Alloys* (Reading, Massachusetts: Addison-Wesley).

Feynman, R., 1954, *Phys. Rev.*, **94**, 262.

Ernst, G., Haug, R. J. Kuhl, J. von Klizing, K., and Eberl, K., 1966, *Phys. Rev. Lett.*, **77**, 4245.

Jancovici, B., and Shiff, D. H., 1964, *Nucl. Phys.*, **58**, 678.

MacDonald, A., 1995, *Les Houches LXI*, 1994, edited by E. Akkermans, G. Montambaux, J. L. Pichard and J. Zinn Justin (Amsterdam: North-Holland).

Stone, M., 1991, *Ann. Phys.* (N.Y.), **207**, 38.

Thouless, D. J., Kohmoto, M., Nightingale, P., and den Nijs, M., 1982, *Phys. Rev. Lett.*, **49**, 405.

Volkov, V. A., and Mikhailov, S. A., 1988, *Soviet Phys. JETP*, **67**, 1639.

Wen, X. G., 1990, *Phys. Rev.* B, **41**, 12 838.