Vorticity quantum numbers for confined electrons

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Abstract. – The eigenstates of a confined particle in an applied magnetic field are characterized by vorticity quantum numbers, defined in a conventional way as gradient of phase integrals on the contour along the boundary line of the sample. The energy spectrum of the problem can be rationalized in terms of diabatic states corresponding to definite vorticity numbers in the whole range of applied fields. The vorticity number of a given state equals the sum of winding numbers of separate, spatially resolved vortices. The vortex patterns evolution shows some surprising similarities with mesoscopic superconductors.

Recent advances in technology have made it possible to fabricate and study micron- and submicron-sized structures which demonstrate plenty of new physical properties as compared to the bulk material [1]. The confined electrons have a discrete energy spectrum. An important feature of nanostructures is the strong influence which the *boundary geometry* has on the energy spectrum of the confined electrons. Thus their eigenstates are characterized by the symmetry point group of the confinement.

On the other hand, the mesoscopic superconductors [2] bring an additional aspect to the physics of nanostructures. The superconducting order parameter, $\psi = |\psi| \exp[i\theta]$, is characterized by the vorticity (or fluxoid) number defined as [3]

$$L = (1/2\pi) \oint_C \nabla \theta \cdot d\mathbf{s}, \quad (1)$$

where C is the contour along the boundary line of the sample [4]. The number L is always an integer because ψ is a single-valued function. It defines the vorticity state, *i.e.* it equals the sum of winding numbers of separate vortices in a given vortex pattern. Therefore, in these systems two kinds of quantum conservation rules are encountered: *symmetry conservation and fluxoid quantisation*. It was recently found that the interplay between these conservation rules gives rise to qualitatively new vortex patterns in mesoscopic superconducting polygons [5].

In this letter we extend the fluxoid quantisation in eq. (1), to confined electrons in applied magnetic fields. We find that the vorticity number plays in this case the role of an additional quantum number, allowing to rationalize the energy spectrum of the confined particles.

To approach this very general problem we will start with a simplified model. Consider an arbitrarily shaped nanosample of a constant thickness in a homogeneous magnetic field applied along the direction perpendicular to the surface of its basis ($\mathbf{H} \parallel \mathbf{z}$). The eigenstates of a single particle of charge e with hard wall confinement are found from the eigenvalue equation:

$$\frac{1}{2m} \left(-i\hbar\nabla - \frac{e}{c}\mathbf{A} \right)^2 \psi = E\psi, \quad (2)$$

under the normal boundary condition on the surface of the sample. Equation (2) corresponds to a quantum billiard model extensively studied experimentally and theoretically [6]. Actually, when the applied field is strong enough the above equation is appropriate to describe electrons in realistic, parabolic confining potentials too. Moreover, in wide structures the confining potential is expected to be flat far enough from the boundaries and therefore the problem can be approximated to some extent with a billiard model also for low values of applied field [7]. In the cylindrical gauge for the vector potential, $\mathbf{A} = \frac{1}{2}\mathbf{H} \times \mathbf{r}$, eq. (2) reduces to two dimensions. The sample can have a symmetry corresponding to a point group C_N , where N is the order of the rotational axis ($\parallel \mathbf{z}$). Then the solutions of eq. (2) are characterized by N different irreducible representations (irreps), *i.e.* transform as

$$\psi_n(\varphi) \sim \exp[in\varphi], \quad n = 0, 1, \dots, N-1, \quad (3)$$

under rotations around the z -axis by symmetry angles, multiple to $2\pi/N$ [8].

Figure 1 shows the lowest part of the spectrum of a square for a negatively charged particle. First, we can see that the whole spectrum can be divided into groups of levels asymptotically approaching one of the Landau levels of the free particle problem, $E_n = \hbar\omega_c(n + 1/2)$ ($\omega_c = |e|H/mc$ is the cyclotron frequency), in the limit of large magnetic fields. Such an asymptotical behaviour is common for quantum billiards of any shape since it arises from the fact that the eigenfunctions shrink with increase of field and feel the boundary less. Second, there is a regular alternation of the symmetry of eigenstates in the spectrum. A square in a homogeneous magnetic field has a symmetry described by the rotational point group C_4 , which contains the irreps A , B , E_+ and E_- with the corresponding numbers $n = 0, 2, 1$ and -1 in eq. (3). One can observe in fig. 1 a periodic repetition of the irreps within the groups of levels approaching each Landau level with the motif A , E_- , B , E_+ . Besides, there is also a periodicity in the symmetry of the lowest level in each asymptotic group. It corresponds to irrep A for the group approaching the lowest Landau level, and further to irreps E_+ for the first-excited, B for the second-excited and E_- for the third-excited Landau level. This behaviour is repeated periodically going to higher Landau levels. Notice that in the spectrum of a positively charged particle the same periodicities are observed, but with E_+ and E_- interchanged.

To have a better insight into this behaviour we calculated the vorticity number of each eigenstate using eq. (1). The results show that L decreases by unity when going to the next level within each asymptotic group in fig. 1. By contrast, the lowest levels in these groups are characterized by L 's increasing by unity when going to the next excited asymptotic Landau level, being $L = 0$ for the ground state. For positively charged particles the two sequences in the spectrum interchange. This actually explains the observed periodicity of the symmetry of eigenstates in fig. 1. Indeed, since for an eigenstate of a given vorticity L the leading angular dependence in the decomposition of the wave function is $\exp[iL\varphi]$, it will transform under the rotations by symmetry angles of the point group C_4 as $\exp[in\varphi]$, where the integer n

Fig. 1 – Energy spectrum of a negatively charged particle in a square in homogeneous magnetic field H as a function of the applied flux $\phi = HS$; S is the area of the square, $\phi_0 = h/|e|c$ is the normal flux quantum and $E_0 = \hbar^2/2mS$.

is taken from the expression $L = n \pmod{4}$. The latter relation gives the correspondence of the vorticity numbers to the irreps, via eq. (3), which is fulfilled by the eigenstates in fig. 1. Interestingly, the same assignment of vorticity numbers to the eigenstates within each asymptotic group also holds in the case of disk-shaped samples. However, while in disks the vorticity number is just the rotational quantum number of the corresponding eigenstate [9], this is no longer the case in square (and other geometry) quantum dots.

The above universal behaviour of the vorticity numbers can be explained further by introducing diabatic states, on the basis of which the spectrum of any quantum dot is easily rationalized. Consider an arbitrarily shaped dot whose boundary is described by a function $r = \rho(\varphi)$, where r and φ are polar coordinates. Consider also a disk with radius a and apply to its eigenfunctions in eq. (2) a transformation of the radial coordinate, $r \rightarrow r'$:

$$r' = \frac{a}{\rho(\varphi)} r. \quad (4)$$

Since r describes the proper (undeformed) space, then the transformed eigenfunctions vanish at $r = \rho(\varphi)$, *i.e.* obey the boundary condition for the quantum billiard with the corresponding boundary line. Using the analytical form of the solutions for disks [9], we can write the new functions in the following form:

$$\psi_{sL}(r, \varphi) = \frac{a}{\rho(\varphi)} C_{sL} e^{iL\varphi} u^{|L|/2} e^{-u/2} M(-\alpha_{sL}, |L| + 1, u), \quad u = \frac{m\omega_c}{2\hbar} \frac{a^2}{\rho(\varphi)^2} r^2, \quad (5)$$

where M is the Kummer function [10], s and L are radial and rotational quantum numbers and

C_{sL} is the normalizing coefficient of the solution for disk. The parameter α_{sL} is determined from the boundary condition $M(-\alpha_{sL}, |L| + 1, m\omega_c a^2/2\hbar) = 0$, defining the quantization of energy levels in disk [9]:

$$E_{sL} = \hbar\omega_c \left(\alpha_{sL} + \frac{1 + |L| - \text{sign}(e)L}{2} \right). \quad (6)$$

The factor $a/\rho(\varphi)$ in the expression for ψ_{sL} was added to provide the orthonormality of these wave functions in the region $r \leq \rho(\varphi)$. Note that although the functions (5) were derived from the solutions for a disk, they cannot be related to the latter by a unitary transformation since these two sets of functions obey different boundary conditions.

ψ_{sL} in (5) are eigenstates of the Hamiltonian

$$\hat{H}' = \frac{1}{\rho} \hat{H} \left(\frac{a}{\rho(\varphi)} r, \varphi \right) \rho, \quad (7)$$

where $\hat{H}$ corresponds to eq. (2). The rhs of (7) implies the coordinate transformation (4) within $\hat{H}$, which is done in a conventional way [10]. Since in r' coordinates $\hat{H}'\psi_{sL}$ coincides with the lhs of the eigenvalue equation (2) for a disk, the eigenvalues of $\hat{H}'(r, \varphi)$ for the boundary condition imposed at $r = \rho(\varphi)$ are just those in eq. (6).

Two important features of the wave functions (5) allow to rationalize the energy spectrum. First, they are characterized by the same vorticity numbers L as the corresponding eigenstates for the disk. The numbers L are actually quantum numbers because the wave functions (5) are also eigenfunctions of the following “vorticity operator”:

$$\hat{L} = -i \frac{1}{\rho} \left(\frac{\partial}{\partial \varphi} + \frac{\rho'_{\varphi}}{\rho} r \frac{\partial}{\partial r} \right) \rho. \quad (8)$$

Second, the eigenvalues (6) follow the common asymptotical behaviour. Actually, by choosing the radius a such that the area of the disk is equal to the area of the arbitrarily shaped sample, the eigenvalues (6) will merge with the corresponding levels of the sample (*i.e.* having the same vorticity number) much faster than the groups of levels merge into degenerate Landau levels. This allows a complete assignment of the energy levels of quantum billiards to diabatic states and explains the universal behaviour of the vorticity numbers in the asymptotic region.

In the opposite limit of small H , the energy levels of low symmetric samples show avoided crossing patterns, corresponding to the mutual repulsion of the states with the same irrep. This is shown in fig. 2 for the lowest part of the spectrum of symmetry A in a square. Each level changes its vorticity number by an integer multiple of four when passing through an avoided crossing region. The reason for such a behaviour becomes clear when the energy level diagram is compared with the scheme of diabatic states levels (dashed lines in fig. 2). Indeed, we can conclude that the avoided crossings pattern arises from the repulsion of diabatic states in the region of their intersections, induced by the perturbation $\hat{H} - \hat{H}'$. The effect of this perturbation increases with diminishing field. On the other hand, in a square the diabatic states belonging to one irrep have vorticity numbers which can only differ by multiples of four (see the discussion above), which explains the corresponding changes of the vorticity numbers in the avoided crossing regions. For quantum dots with a rotational symmetry axis of order N , the vorticity number of a given level will change with the field by a multiple of N .

Further investigations provided evidence for a vortex structure of the obtained solutions for quantum billiards (fig. 1) in striking analogy with the vortex states found in mesoscopic superconductors [2, 5]. By applying eq. (1) locally to different regions of the sample it is

Fig. 2 – Low-energy region of the spectrum of eigenstates of symmetry A (full lines) and the corresponding diagram of diabatic states levels (dashed lines). Vorticity numbers are indicated at each level.

Fig. 3 – Gradient of phase plots corresponding to the first-excited state of symmetry A at three values of applied flux (a, c, d), shown by squares in fig. 2, in the region of avoided crossing. Panel b is the $|\psi|^2$ distribution corresponding to the state in a ; dark regions indicate the low density.

confirmed that, as in the case of mesoscopic superconductors, the vorticity number in a given eigenstate equals the sum of winding numbers of separate, spatially resolved vortices. Vortex patterns are consistent with the symmetry of the confinement, which in the case of a square implies their following structure:

$$L = n + \sum_{i=1}^m 4L_i, \quad (9)$$

where n is the winding number of the vortex in the centre, matching the number in eq. (3) of the corresponding irrep, and m is the number of quartets of normal vortices ($L_i = \pm 1$) forming transitive sets under C_4 rotations. These patterns change continuously with the applied field except for avoided crossing regions corresponding, in the case of a negative particle, to the *entry/exit of antivortices* ($L = -1$). Symmetry requirements allow antivortices to cross the boundary line only by four via middle edges and corners or by eight (four symmetric pairs) via edges. Therefore vorticity changes generally in several jumps when $|\Delta L| > 4$ at the avoided crossing. Figure 3 shows the evolution of the vortex pattern in the second state of symmetry A when passing through the first avoided crossing region. At low field (*a*) the pattern consists of four vortices and four antivortices, giving the total $L = 0$. Approaching the centre of the avoided crossing, the four vortices move towards the edges. Concomitantly, four antivortices enter via edges (*c*) and then annihilate with the four vortices leaving finally four antivortices on diagonal positions and the total $L = -4$ (*d*). In the upper state of this avoided crossing, the third state of irrep A (fig. 2), vorticity is $L = -4$ at low fields (four antivortices on axial positions). In the centre of the avoided crossing four vortex-antivortex pairs nucleate spontaneously on the diagonal positions, then four antivortices from these pairs exit via corners at higher fields, leaving the pattern “4 axial antivortices + 4 diagonal vortices” ($L = 0$).

This scenario seems to be general for states of all symmetries, at least in the low-energy part of the spectrum: increasing the field, antivortices *always enter* and only *via edges* in the lower state, while they *always leave* the sample in the upper state, one of the steps always including the exit *via corners* at each avoided crossing. The lack of mirror symmetry of the vortex pattern evolution in the lower and the upper state means that avoided crossing regions are badly approximated by two interacting levels, which seems surprising in the view of a satisfactory description of the spectrum by diabatic states (fig. 2). In the asymptotic region, the vortex patterns in the states corresponding to the ground Landau level evolve to structures where all m quartets of vortices in eq. (9) are situated on diagonal positions, which mimics well the vortex patterns in mesoscopic superconducting squares close to the phase boundary [11]. This is another surprise since the particle wave function in quantum billiards and the order parameter in superconductors obey entirely different boundary conditions. On the other hand, the vortex patterns in the states belonging to the first-excited Landau level correspond to the states from the ground Landau level superimposed on a common structure “four axial antivortices + 4 diagonal vortices”. This background structure forms a ring of lowered density, seen already in the lowest states (fig. 3b), which is reminiscent of the radial node line in the wave function of the first-excited Landau level. The obtained patterns can be observed experimentally by measuring the $|\psi(\mathbf{r})|^2$ maps in scanning tunnelling spectroscopy [12].

In conclusion, vorticity numbers for confined electrons and their interplay with symmetry conservation quantum numbers have been investigated within the quantum billiard model. The energy spectrum is rationalized in terms of diabatic states for which vorticity numbers are quantum numbers in the conventional sense. The particle eigenstates are characterized by a vortex structure which underlies the corresponding vorticity number and shows surprising similarities with mesoscopic superconductors.

Given the general character of the results, they are expected to show up in real nanostructures, quantum dots [13]. For a realistic description of such systems further refinements concerning the one-electron confining potential and the interelectron interaction [14] should be taken into account.

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