Localization, Wave-Function Topology, and the Integer Quantized Hall Effect

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In a magnetic field, a wave function in a two-dimensional system is uniquely specified by the position of its nodes. We show that for high fields and a weak random potential, motion of the zeros of the wave function under smooth changes of the boundary conditions can be used to characterize the behavior of the one-electron states and distinguish between localized and extended states.

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Following the discovery of the quantized Hall effect[1] an argument for the quantization based on gauge invariance was given by Laughlin,[2] which also shows that changes in σ_{xy} can occur only if the Fermi energy lies in a region of extended states. Further work by Thouless and co-workers[3] and others[4-6] has related the quantized value of σ_{xy} to topological properties of wave functions; from this viewpoint, the connection with delocalization of the wave function is not clear. In this paper, we show that a simple connection between delocalization of wave functions and their topological characteristic which leads to a nonzero σ_{xy} can be made. The existence of truly delocalized states in the large field limit is to be contrasted with the behavior of 2D systems at $H=0$ where no extended states are believed to exist.

In the presence of a magnetic field, wave functions exhibit nodal points rather than nodal lines, the latter being the generic situation in systems with time reversal symmetry. In two dimensions, and in a high enough magnetic field that the electrons can be considered confined to the lowest Landau level (LLL), wave functions are *completely* determined by the location of their zeros. Such a description provides a convenient and physical approach to understand localization produced by a disordered single-body potential. When generalized periodic boundary conditions are enforced over a finite system, the zeros, now finite in number, move smoothly under continuous changes in the boundary conditions. The sensitivity of a wave function to boundary-condition changes allows a distinction between localized and extended states[7]; we shall show that there exist states whose wave function can be forced to vanish at *any* specified point in real space by a suitable choice of boundary conditions. Such a state naturally appears to be "extended"; moreover, the covering of real space by the zeros of the state is characterized by an integer, which is identical to the quantized value of the boundary-condition averaged σ_{xy}.

We consider the Hamiltonian $H=H_0+V(\mathbf{r})$ in two dimensions, with kinetic energy $H_0=(2m)^{-1}(\mathbf{p}+e\mathbf{A}/c)^2$. We work in an arbitrary gauge $\mathbf{A}=\frac{1}{2}\mathbf{r}\times\mathbf{B}+\hbar c/e\Delta\chi$, with $\mathbf{B}=-B\hat{\mathbf{z}}$ the magnetic field. For a free particle, H_0 is a harmonic oscillator in the cyclotron coordinates, with a spectrum $E_n=(n+\frac{1}{2})\hbar\omega_c$ and a natural cyclotron frequency $\omega_c=eB/mc$. Each Landau level is extensively degenerate, with a density of states per unit area $N_s/\Omega=1/2\pi l^2$, where $l=(\hbar c/eB)^{1/2}$ is the magnetic length. When an external potential $V(\mathbf{r})$ is imposed, the Landau levels will both broaden and mix; however, when the cyclotron frequency is sufficiently large, the essential physics is well described by a LLL-projected Hamiltonian. (We assume that the LLL is only partially occupied, i.e., $\nu=2\pi l^2 n<2$, where n is the areal density). The most general form of a LLL wave function is

$$\psi(\mathbf{r})=f(z)e^{-z\bar{z}/4l^2}e^{-i\chi}, \tag{1}$$

where $z=x+iy$, and $f(z)$ is an analytic function of its

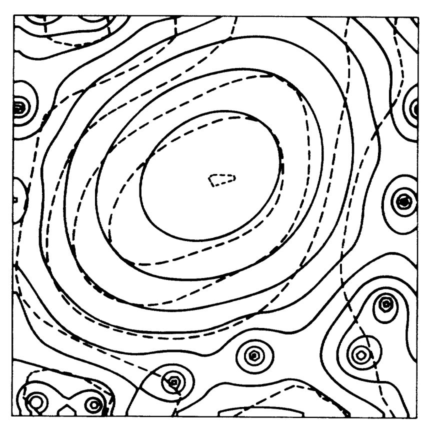

FIG. 1. Contour maps (in the primitive unit cell) of a numerically generated smooth random potential (dashed lines, linear scale), and of the probability density $|\psi_8|^2$ of the highest-energy state (solid lines, logarithmic scale).

argument. In order to treat finite systems, we impose generalized periodic boundary conditions on a square of side L containing an integral number of flux quanta $N_s = L^2/2\pi l^2$, by requiring $t(\mathbf{L}_j)|\psi\rangle = e^{i\theta_j}|\psi\rangle$ $(j=1,2)$, where $t(\mathbf{r})$ is the magnetic translation operator.[8] This leads to a general form for f (in terms of the rescaled length variable $\xi = z/L$)

$$f(\xi) = e^{\pi N_s \xi^2/2} e^{2\pi i\lambda\xi} \prod_{k=1}^{N_s} \Theta_1(\pi(\xi-\xi_k)\,|\,i), \tag{2}$$

where $\Theta_1(\omega\,|\,\tau)$ is the Jacobi Θ function, which possesses simple zeros at $\omega/\pi = j_1 + \tau j_2$ for all integers j_1, j_2. The freedom to choose arbitrary boundary-condition phases θ_1, θ_2 follows from the breaking of time-reversal symmetry by the magnetic field; fixing the θ_j leads (for N_s even) to the condition $\lambda = n_1 + \theta_1/2\pi$ as well as a constraint on the "center-of-mass" coordinate

$$\xi_{\text{c.m.}} = N_s^{-1} \sum_{k=1}^{N_s} \xi_k = N_s^{-1}\left[(n_2 + \theta_2/2\pi) - i\lambda\right].$$

Here n_1, n_2 are integers, each of which may take on N_s distinct values, $0 \le n_j < N_s$. (For N_s odd, one replaces n_j by $n_j + \frac{1}{2}$ in the above formulas.) Equation (2) shows that there will be precisely N_s zeros inside the principal region Ω $[0 \le \mathrm{Re}(\xi) < 1;\ 0 \le \mathrm{Im}(\xi) < 1]$ which are

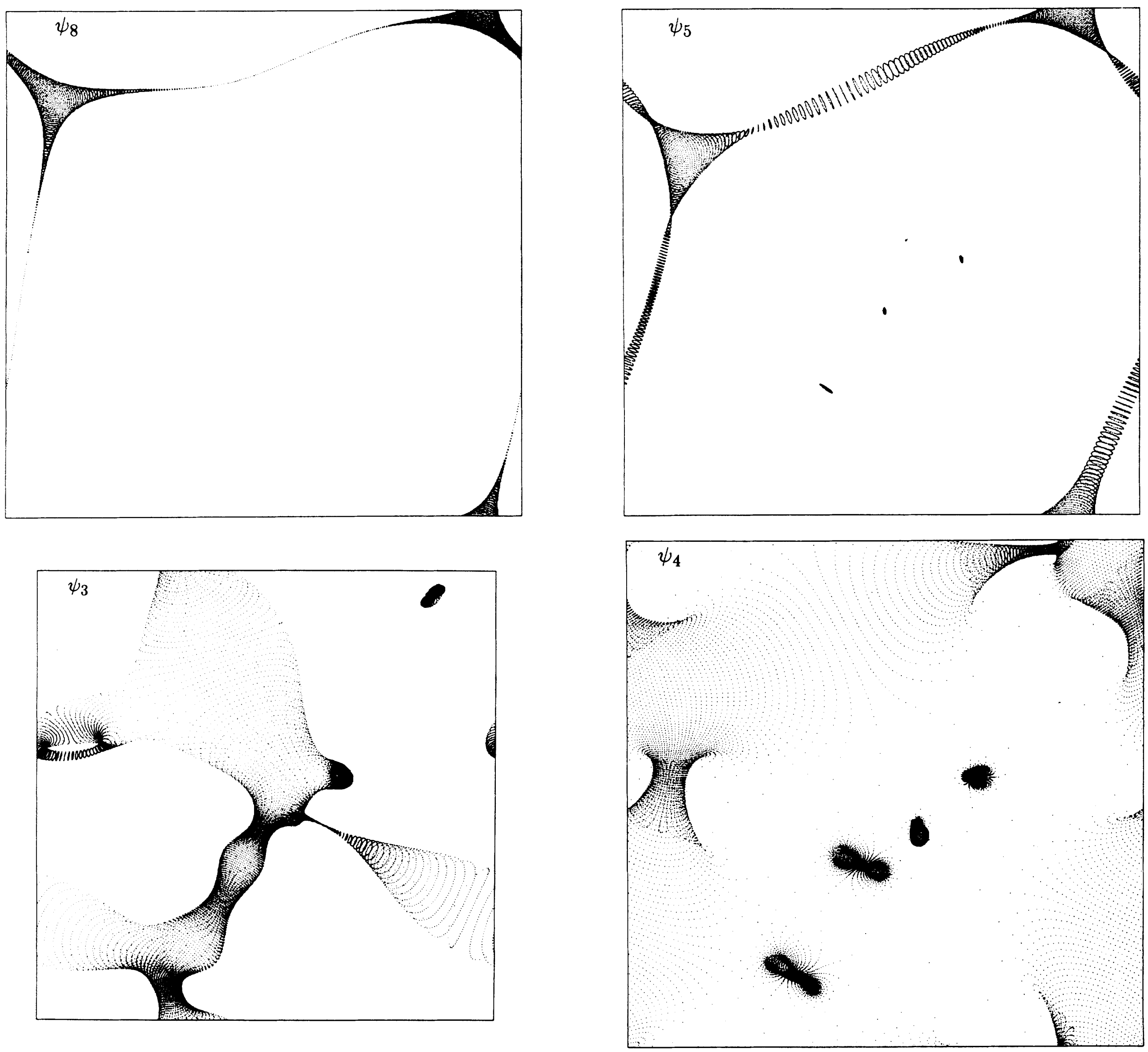

FIG. 2. Map of the nodal points of four of the $N_s(=8)$ wave functions in the potential of Fig. 1 for a fine grid of boundary conditions.

periodically repeated in every unit cell. The position of the zeros ξ_k *completely* determines the wave function. There are precisely N_s states, which are nondegenerate for a general potential $V(\mathbf{r})$, and are quasiperiodic, satisfying

$$\psi(\mathbf{r}+\mathbf{L}_j)=e^{i\theta_j}\exp(i\mathbf{r}\times\mathbf{L}_j\cdot\hat{\mathbf{z}}/2l^2)\psi(\mathbf{r}).$$

In Fig. 1, we show a contour plot of a typical smooth potential $v(\mathbf{r})$ (with a correlation length chosen equal to the magnetic length) together with a contour plot of $\log|\psi|$ for the highest energy state ψ_8 for $N_s=8$. The wave function is peaked on the hill of the potential, and the eight zeros cluster along the potential minima as would be expected on semiclassical grounds.[9] We now study the sensitivity to boundary conditions by plotting (Fig. 2) the location of the zeros for four of the eight states in the potential of Fig. 1, for a fine mesh of points covering the boundary angle space $0\le\theta_j<2\pi$. Each zero moves smoothly as the values of θ_j are continuously changed. For the state ψ_8, the zeros move along fine filaments connecting around the real-space torus. That the pattern of zeros must be connected in this fashion follows from the constraint on $\xi_{\text{c.m.}}$ and the periodicity of the zeros under $\theta_j\to\theta_j+2\pi$.

With decreasing energy, the states $\psi_{7\text{-}5}$ possess similar filamentary structure, which broadens slightly as the center of the band is approached. In addition, there appear nodes on the hill of the potential which are insensitive to the boundary conditions; they correspond to the semiclassical description of localized states of increasing angular momentum centered on the hill.[9] Thus the state ψ_5 has three "localized" zeros. A similar picture applies to the low-lying states $\psi_{1\text{-}2}$, with the wave function now predominantly confined to the potential minimum (although a semiclassical description is less appropriate because the minimum of the potential in Fig. 1 is less pronounced than the maximum). ψ_3 is on the verge of delocalization, but the zeros remain confined to a bounded region of the torus.

The fourth-highest state ψ_4 departs radically from this picture. The zeros are now highly mobile, and completely cover the real-space torus, although their density is far from uniform. Such extreme sensitivity to boundary conditions is characteristic of the behavior of an extended state[7], and we believe it may be used as a definition: An extended state may be made to vanish at any specified point by a suitable choice of the θ_j. All states can be characterized by a relative integer, the Chern index $C_1(m)$, which counts the covering of the real-space torus by the zeros $\xi_k(\theta_1,\theta_2)$ for the state ψ_m. $C_1(m)$ takes the value +1 for $m=4$ and is zero for the remaining states in Fig. 2. This is easily seen if one notes that the zero maps of Fig. 2 are, with the exception of ψ_4, projections of "tubes," so that the inverse map of zeros in θ space for fixed ξ is typically null or double valued. It is straightforward to show that $\sum_{m=1}^{N_s}C_1(m)=1$, so that there must exist at least one nontrivial state.

We have also calculated the Hall conductivity σ_{xy} as a function of both energy ϵ and boundary-condition angles. The Kubo formula may be written as[3]

$$\sigma_{xy}(E;\theta_1,\theta_2)=\sum_{m=1}^{N_s}\delta\sigma_{xy}(m;\theta_1,\theta_2)\Theta(E-E_m),$$

$$\delta\sigma_{xy}(m;\theta_1,\theta_2)=\frac{1}{2\pi i}\frac{e^2}{h}\epsilon_{ij}\frac{\partial}{\partial\theta_i}<\tilde{\psi}_m\,|\,\frac{\partial}{\partial\theta_j}\,|\,\tilde{\psi}_m>, \tag{3}$$

$$|\,\tilde{\psi}_m> =\exp[-i(x\theta_1+y\theta_2]\,|\,\psi_m>,$$

where E_m is the energy of state ψ_m. As demonstrated by Thouless and co-workers,[3] the unweighted average of $\delta\sigma_{xy}(m)$ over all boundary angles is necessarily an integral multiple of e^2/h. This integer can be identified as $C_1(m)$, so that only the state ψ_4 in Fig. 2 has a nonzero boundary-condition averaged Hall conductance, as we have checked by direct numerical calculation. $C_1(m)$ is an invariant (the first Chern character) characterizing the vector bundle (the set of zeros ξ_k) over the torus. Intuitively the relationship between space-covering zeros and the boundary averaged $\delta\sigma_{xy}$ is clear, because a nonzero value of C_1 can arise only if there is ambiguity in our fixing the phase of the wave function $\psi_m(\mathbf{r},\theta_1,\theta_2)$ over the whole space of boundary angles.[10] The bundle is trivial (and $C_1=0$) provided one can fix the phase of the wave function at some fiducial point $\mathbf{r}_0$ so that $\psi(\mathbf{r}_0,\theta)$ is real and positive for all θ; this is possible provided there exists an $\mathbf{r}_0$ such that $\psi(\mathbf{r}_0,\theta)$ never vanishes. For the states in the potential of Fig. 1 (four of which are shown in Fig 2), only for ψ_4 does a global choice of

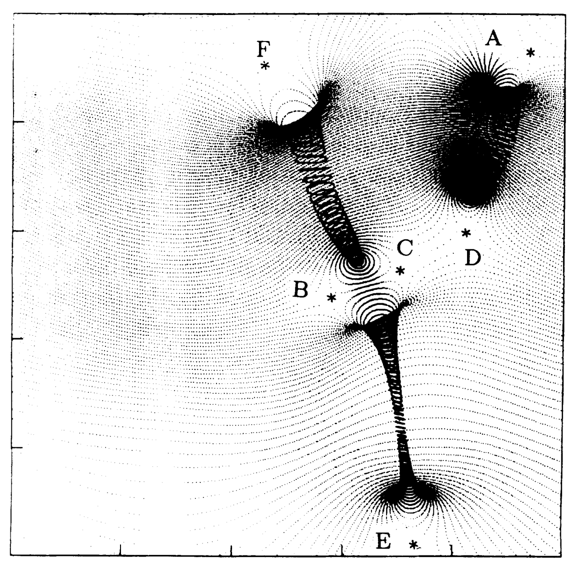

FIG. 3. Zero map of a state of Chern character +1 for $N_s=4$. The positions of the six double zeros are shown.

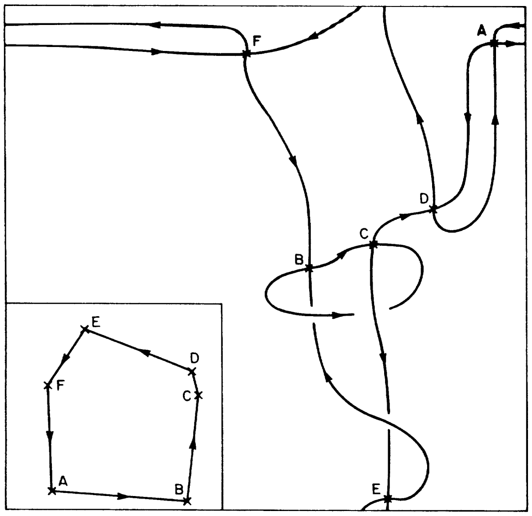

FIG. 4. Topology of the braiding of zeros associated with the closed path ABCDEFA in boundary-angle space (inset).

$\mathbf{r}_0$ not exist.

More understanding of the character of the wave functions can be obtained by the study of the braiding of paths of the zeros $\xi_k(\boldsymbol{\theta})$ under continuous paths in $\boldsymbol{\theta}$. We have found the existence of double zero ξ^* at isolated points $\boldsymbol{\theta}^*$ to be a generic occurrence for all wave functions in the band.[11] For $\boldsymbol{\theta}$ close to $\boldsymbol{\theta}^*$ the two nodes (labeled here ξ_j,ξ_k) will be distinct; under a path which circuits $\boldsymbol{\theta}^*$ (anticlockwise, say) and returns to the initial point, the two zeros will orbit each other (either anticlockwise or clockwise, i.e., with sign ± 1) and interchange. The point ξ^* is a branch point at the intersection of two sheets of the N_s-valued function $\xi(\boldsymbol{\theta})$; close to $\boldsymbol{\theta}^*$, two of the zeros are given by solutions of

$$(\xi-\xi^*)^2=K_1(\theta_1-\theta_1^*)+K_2(\theta_2-\theta_s^*),$$

with $K_{1,2}$ complex constants. Because the base space is a torus, the number of double zeros is even.

We have analyzed a state of Chern character $+1$ for the case $N_s=4$. The zero map for this state is shown in Fig. 3, together with the location of the six double zeros $\xi^*_{\text{A-F}}$. The value of C_1 can be determined directly from the topology of the knot produced by the motion of the zeros under the closed noncrossing path $\boldsymbol{\theta}^*_{\text{A}} \to \boldsymbol{\theta}^*_{\text{B}} \to \cdots \boldsymbol{\theta}^*_{\text{F}} \to \boldsymbol{\theta}^*_{\text{A}}$ (Fig. 4). The knot consists of lines joining the points ξ^*, with two trajectories entering, and two leaving each vertex. Those points (in real space) interior to any closed loop can be "covered" by a single zero, by contraction of the corresponding loop in boundary-angle space to a point. If there are no exterior points (which is the case of Fig. 4, because the knot is connected around the torus in both directions) the Chern character will be nonzero. If the knot is homotopic to a point, then $C_1=0$. A more detailed discussion of the braiding of zeros and the associated monodromy structure will be discussed in a forthcoming paper.[12]

To conclude, we have shown that studying the sensitivity of nodes of the wave function to changes in boundary conditions can be used to differentiate the behavior of localized and extended states. An extended state may be forced to vanish at any specified position in real space by the appropriate choice of boundary conditions. This nontrivial topological structure leads in particular to a nonzero Hall conductance.

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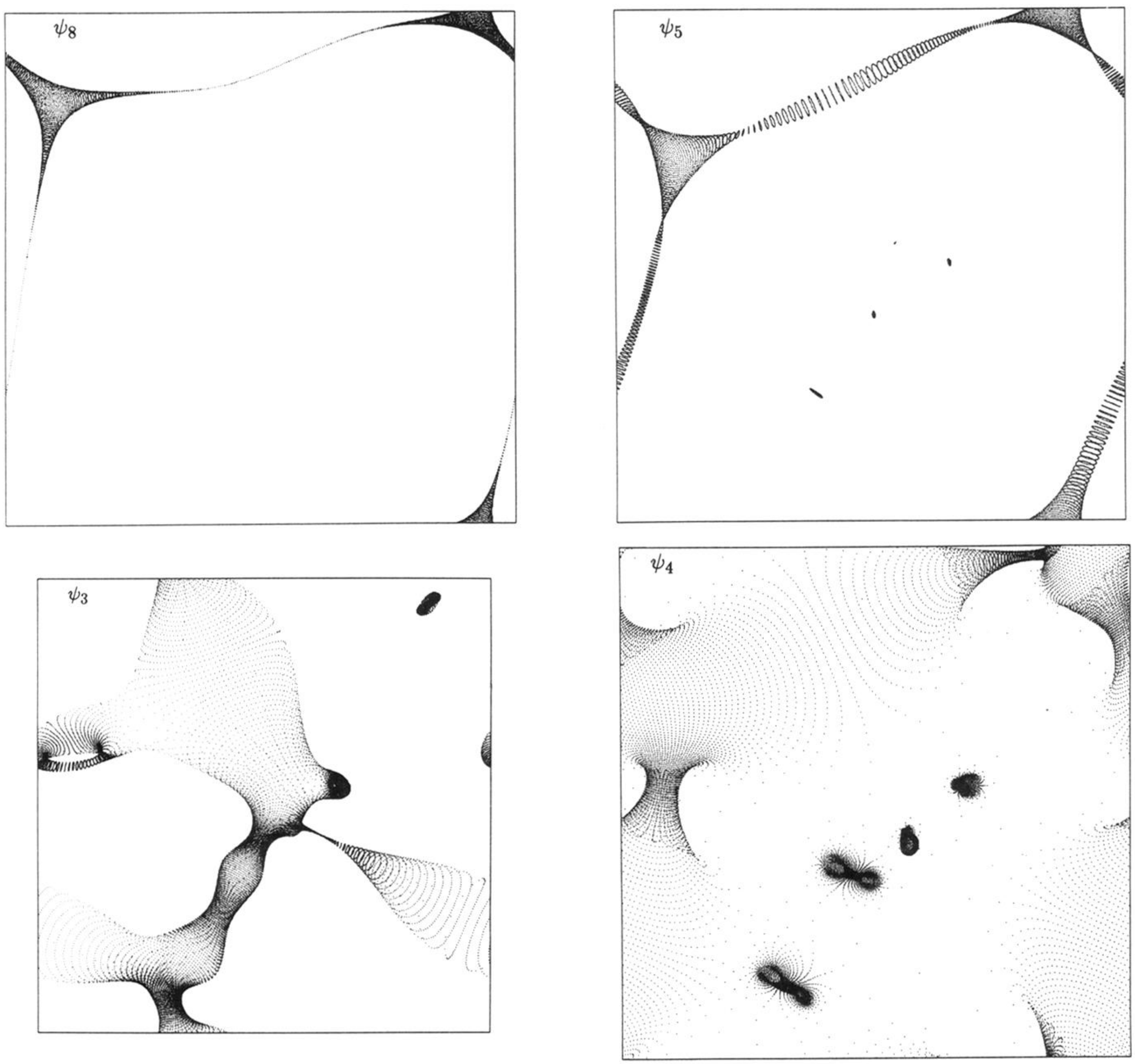
[11]In contrast to the analytic dependence of f on $\xi=\xi_1+i\xi_2$, there is no such analyticity as a function of any combination $\theta=\theta_1+\tau\theta_2$. Therefore, we denote the pair (θ_1,θ_2) by $\boldsymbol{\theta}$.

[12]D. P. Arovas, R. N. Bhatt, F. D. M. Haldane, P. B. Littlewood, and R. Rammal, to be published.



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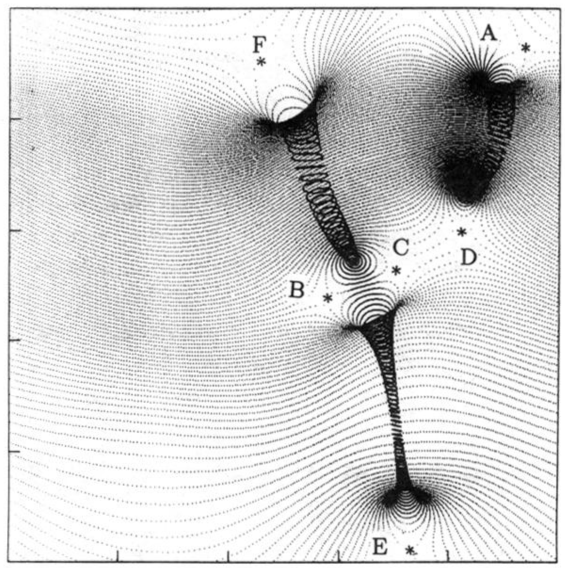

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