Localization by interference: Square billiard with a magnetic flux

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Eigenstates and energy levels of a square quantum billiard in a magnetic field, or with an Aharonov-Bohm flux line, are found in quasiclassical approximation, that is, for high enough energy. Explicit formulas for the energy levels and wavefunctions are found. There are localized states, never before noticed in this well studied problem, whose localization is due to phase interference, even though there is no or negligible classical effect of the magnetic field. These and related states account almost entirely for the magnetic response in certain temperature ranges, and thus have a bearing on the experiments of Lévy, et al.

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The problem of a quantum charged particle subject to a magnetic flux and confined in two dimensions, say to a square billiard, has attracted much attention. The simplest fluxes are (1) a uniform magnetic field [UF] and (2) an Aharonov-Bohm flux line [ABFL]. One motivation for (1) is experimental mesoscopic physics. Lévy, et al. have made theoretically resistant[6] measurements of the magnetic susceptibility of an array of such squares. Clearly, such a simple problem should be added to the physicist’s arsenal of known results.

The Aharonov-Bohm flux line[7] has had a rather spectacular effect on physics. It provides a compelling example of quantum nonlocality. Largely because of this example, it is now clearly understood that charged quantum particles have phase interference effects originating from a magnetic field that vanishes in all regions accessible to the particle. Although this purely quantum effect has no directly corresponding classical physics, it is related to the scattering of a classical charge neutral wave from a vortex[8]. Aside from this conceptual motivation, an ABFL is a simple idealized extreme case, which like the uniform field should be thoroughly understood as there are numerous applications. For example, Laughlin’s explanation[9] of the quantum Hall effect is based on ABFL physics.

Another reason for interest is that a magnetic flux is the most obvious way to break time reversal symmetry of simple systems like billiards[10]. The finite flux case is in a different universality class from the zero flux case. This has inspired much numerical work[11]. Also, square symmetry conflicts with the apparent circular symmetry of the flux. This, as for the Sinai billiard, suggests chaos[12]. Indeed, the circular billiard in a uniform field is relatively trivial and uninteresting.

Thus, much work has been devoted to these systems. It is surprising that there is something new, simple and interesting to say about square billiards with a flux.

We here present some analytic results with numerical confirmation. The results are possible because we exploit two small parameters. First, we treat the particle quasiclassically, that is, its wavelength is short compared with the system parameters. Second, we treat the field classically weak, which is automatic for the ABFL. For the UF, we assume that \( \epsilon = L/R_c \) is small, where \( L \) is the square side and \( R_c \) is the cyclotron radius.

Nearly all previous work has focused on level statistics, or smoothed state densities. In contrast, we find analytic wave functions, and simple formulas for their energies. The unexpected result is that an important class of these eigenstates are localized. Unlike the eigenstates of the flux-free case, which uniformly fill the square, some of the eigenstates have support in a small fraction of the square. The area of this support vanishes at infinite energy. Associated with a given extremely localized state is a sequence of states which progressively become more delocalized, but which share with the localized state a simple structure. The most prominent such sequence dominates the magnetic susceptibility in the UF case, as measured by Lévy.

This localization, like Anderson localization[13], is caused by phase interference. A bunch of classical phase space points mimicking a wave packet in a disordered two dimensional region, or in a square, will spread, diffusively in the disordered case, linearly in the square, and eventually become uniformly distributed. Taking into account the phases in impurity scattering, or from the magnetic flux, leads to interference effects that suppress the wave packet spreading. Many interesting effects of the ABFL have been discovered in the last forty years, but we have found no previous work that produces a localized quantum state through destructive ABFL interference.

In this paper we shall not discuss to its conclusion the ideal zero radius ABFL. That limit best establishes quantum nonlocality, but quantum nonlocality is no longer disputed. We have found that the zero radius limit leads to interesting but distracting mathematical and numerical problems. Basically, there are diffraction effects which complicate the results. In this paper we want to avoid that issue in favor of understanding the main phase interference effect. We therefore eventually endow the flux line with a finite radius \( \rho \) whose scale we discuss later. Initially, however, we suppose \( \rho = 0 \).

For UF, the cyclotron radius is \( R_c = v/\omega_c = cp/eB \), where \( \omega_c = eB/mc \) and \( p = mv \). The momentum \( p = \hbar k = h/\lambda \) is related to wavenumber \( k \) and wavelength \( \lambda \). Then \( \epsilon = L/R_c = eBL/\hbar c = 2\pi\phi/\phi_0kL \). Here \( \phi \) is the magnetic flux \( BL^2 \), and \( \phi_0 \) is the flux quantum \( hc/e \). This expression carries over to the ABFL if we identify \( \phi \) with the flux in the flux line. For the ABFL \( \phi \) may as well take \( |\phi/\phi_0| \leq 0.5 \), but for the UF \( \phi \) can be large as long...
as $\epsilon$ is small. We choose units such that $B = 2\pi \Phi/\phi_0$ and $L$, $\hbar$ and $2m$ are unity, so that $\epsilon = B/k$. We also suppose $k > 1$, justifying the quasiclassical approximation.

Our approach utilizes the quasiclassical surface of section [SS] method of Bogomolny. His operator $T(x, x'; E)$ takes the electron crossing the SS at point $x'$ to its next crossing at $x$, all at energy $E = k^2$. The SS can be chosen in many ways. To simplify $T$, we use a method of images. Namely, we consider, instead of a unit square, $x, y \in [0, 1] \otimes [0, 1]$, an infinite channel of width 2 obtained by reflecting the original square first about $x = 0$ and then about $y = 1$, and finally repeating the resulting $2 \times 2$ square periodically to $|x| = \infty$. The flux changes sign in neighboring squares. The solutions to the square are found from the channel solutions by using symmetry, e.g., the solution odd under $y \leftrightarrow 2 - y$ corresponds to Dirichlet conditions at $y = 1$.

The SS is taken as the axis $y = 0$ which is identified with $y = 2$. This gives

$$T(x, x'; E) = \left( \frac{1}{2\pi i} \left| \frac{\partial^2 S(x, x'; E)}{\partial x \partial x'} \right| \right)^{\frac{1}{2}} \exp(iS(x, x'; E)).$$

(1)

Here $S = \int p \cdot \mathbf{dr}$ is the action integral along the classical path from $(x', 0)$ to $(x, 2)$. Because the field is classically weak, this path is approximated by a straight line. We immediately find

$$S(x, x') = k \sqrt{4 + (x - x')^2} + \Phi(x, x'),$$

(2)

the flux free result plus $\Phi = (e/c) \int \mathbf{A} \cdot d\mathbf{r}$.

Periodic orbits on the square correspond to straight line orbits in the channel from $(x', 0)$ to $(x = x' + 2p/q, 2)$. Here $p$ is a positive integer and $q$ is a positive or negative integer relatively prime to $q$. Negative and positive $p$ are not equivalent if there is a magnetic flux. Such orbits correspond to a $(p, q)$ classical resonance which is strongly affected by a perturbation.

Our scheme finds solutions of $T\psi = \psi$ by a perturbation theory. We first solve $\int T(x, x')\psi(x') = e^{i\omega(k)}\psi(x)$, treating $k$ as a parameter, and then find the energies by solving $\omega(k) = 2\pi n$. Given $\psi(x)$, a quadrature yields the full wave function $\Psi(x, y)$. Given $\Psi$, for billiards $\Psi(x) \propto \partial \Psi/\partial n \propto \partial \Psi(x, y)/\partial y|_{y=0}$.

Specializing to the $(1,1)$ resonance we look for a solution $\psi(x) = e^{i\omega}u_m(x - 1/2)$, where $\kappa = k \cos 45^\circ$, and $u_m$ varies much more slowly than the exponential. The rapidly varying phases in the integral $\int T\psi$ are stationary at $x' = x - 2$. This corresponds to diamond shaped periodic orbits of the original square whose sides make angles of $45^\circ$ with the $x$ axis. It suffices to evaluate $\Phi(x, x')$ at $\Phi(x, x - 2) = \Phi(x + 2, x)$. This is equivalent to integrating the vector potential about the closed diamond loop, and so is independent of gauge. The result is that $u_m$ satisfies the Schrödinger equation

$$-u'' + V(x)u_m = E_m u_m,$$

(3)

where $V(x - 1/2) = -k\Phi(x + 2, x)/\mathcal{L}$, and $\mathcal{L} = \sqrt{8}$ is the length of the diamond orbits. Thus we convert the phase $\Phi$ to a ‘potential’ $V$. For UF,$$

V(x) = -Bk(\frac{1}{2} - 2x^2)/\mathcal{L}; \ x \in [-\frac{1}{2}, \frac{1}{2}],

V(x) = +Bk(\frac{1}{2} - 2(x + 1)^2)/\mathcal{L}; \ x \in [-\frac{3}{2}, -\frac{1}{2}],

V(x) = V(x + 2).

(4)

For the $(-1,1)$ resonance, whose orbits are time reversed $(1,1)$ orbits, $V(x)$ changes sign. This would not be true if $V$ had its origin in a time reversal invariant perturbation of the square, for example, a small change of shape. Note also that this periodic extension of the $x$ coordinate is similar to use of a ‘angle’ variable, with positive $x$-velocity $v_x$ for $x \in [0, 1]$, and negative $v_x$ for $x \in [1, 2]$.

For ABFL, we must choose where to put the flux line. The square center offers some numerical convenience, but the results are not very interesting. We place the line at $(\frac{1}{2}, a)$ which still gives some symmetry and is readily compared with the UF case. Then

$$V(x) = -Bk/\mathcal{L}; \ x \in [-a, a],$$

$$V(x) = +Bk/\mathcal{L}; \ x \in [-1 - a, -1 + a],$$

(5)

and for other points in $[-\frac{3}{2}, \frac{1}{2}], V(x) = 0$. This ‘square well’ potential is also continued periodically. Strictly speaking, this potential, because of the steps, varies too rapidly for the theory to apply. We will modify it below.

It’s clear that $Bk$ is the important parameter in the UF case, while for the ABFL, both $Bk$ and $a$ are important. For sufficiently large $Bk$, Eq. (5), in the UF case, will have low lying tight binding harmonic oscillator type solutions centered at $x = 0$ (if $B > 0$), with energies

$$E_m = -\frac{1}{2}Bk/\mathcal{L} + (m + \frac{1}{2})\sqrt{8Bk/\mathcal{L}}.$$  

(6)

The lowest wave function is approximately $u_0(x) = e^{-\sqrt{Bk/2}\mathcal{L}^2}x$ which is arbitrarily narrow at large energy.

For the ABFL

$$u_{m-1}(x) \approx \sin \left( m\pi(x + a)/(2a) \right); \ |x| < a$$

$$\approx 0; \ |x| > a$$

(7)

and the energy is

$$E_m \approx -Bk/\mathcal{L} + (m + 1)^2 \pi^2/4a^2.$$  

(8)

Here the width of the state $u$ is determined by $a$, and the tight binding approximation will be good provided $Ba^2k/\mathcal{L} >> 1$. The localization of these states in $x$ leads to the localization of the full state in the square. The total energy is given approximately by

$$k_{n,m} = 2\pi n/\mathcal{L}E_m/k.$$  

(9)

Eq. (8) should be solved iteratively. For example, the first approximation replaces the $k$ dependence of the term $E_m/k$ by $2\pi n/\mathcal{L}$. Equivalently, the energy $E_{n,m} = 4\pi^2n^2/\mathcal{L}^2 + 2E_m$. 


We next give an expression for \( \Psi(x, y) \), shifting the origin to the square center:

\[
\Psi_{nm}(x, y) = \left( \sum_{s=0}^{3} i^{-rs} R_s \right) e^{i\frac{\pi}{2} (x+y)} u_m(x - y - \frac{1}{2}).
\]

(10)

Here \( R : (x, y) \to (y, -x) \) is the rotation by 90°. The UF Hamiltonian can be taken to be invariant under \( R \), while the approximations made for the ABFL induces this invariance. Here \( r \) labels the rotational symmetry of the wave function, i.e. \( R = i^r \). Another symmetry gives \( u_m(x) = (-1)^m u_m(-x) \). The symmetry under translation is \( u(x + 2) = (-1)^r u(x) \). The relation is

\[
r = -n \mod 4 + 2(1 - m \mod 2).
\]

(11)

Thus Eq. (10) holds for all symmetries and successive values of \( n \) cycle through the representations of \( R \).

It is easily checked that the \( \Psi_{nm} \) vanishes on the square sides. This wave function can also be obtained as a kind of Born-Oppenheimer or channelling approximation. To see that \( \psi_m \approx \partial \Psi/\partial n \), just observe that the derivative, say \( \partial/\partial y \) at \( y = -\frac{1}{2} \), need be applied only to the rapidly varying exponential.

Fig. 1. shows numerically calculated \(|\Psi(x, y)|\), which is gauge invariant, for \( n = 62, k \approx 2\pi n/2 \approx 118, m = 0, B = 25, \sqrt{B/\rho} \approx 59 \). Current density for the same state is shown in Fig. 2. For such a well localized \( u_m \), each term in Eq. (10) dominates one side of the diamond orbit. In this case \(|\psi_m| \approx |u_m| \). There is interference near the square’s edges, so the first maximum of \(|\Psi| \) (e.g. near \((0, \pm \frac{1}{2})\)) is about twice as large as \(|\Psi(\pm \frac{1}{2}, \pm \frac{1}{2})|\). The current density is thus largest close to the middle of the square’s edges. These states are paramagnetic, that is, their current circulates in the opposite sense from that of a free particle in the field.

There is no localized state in the time reversed sense. However, the states with \( m \) of order \( \sqrt{B/\rho} \), corresponding to \( E_n \sim +Bk/2L \), energetically at the top of ‘potential’ \( V(x) \), are diamagnetic. This actually corresponds to the (1,1) resonance. These states are not spatially localized, although they do have a sort of localization in momentum space, as we show in the next paragraph. More generally, as \( m \) increases, the states become more delocalized, and eventually become independent of \( B \). This means that for larger \( m \) all four terms in Eq. (10) make comparable contributions at an arbitrary typical point \( x, y \), whereas in the localized case, one or two terms contribute. This gives interference oscillations in \(|\psi_m| \) near \(|x| \approx \frac{1}{4} \) as shown in Fig. 3b.

We have assumed that \( n > m \), and that \( u_m \) is slowly varying compared with \( e^{i\pi n x/2} \). Expanding, \( u_m = \sum \tilde{u}_{m,l} e^{i\pi l x/2} \), where \( 2l \) is an integer satisfying \((-1)^{2l} = (-1)^l \). Also \( \tilde{u}_{m,l} = (-1)^m \tilde{u}_{m,-l} \). The unperturbed states can be labelled \( p,q \) with unperturbed energies \( \epsilon_p^2 + q^2 \), dropping the factor \( \pi^2 \). For \( r \) even, Eq. (10) is a superposition of unperturbed states with quantum numbers \( p = \frac{1}{2} n + l, q = \frac{1}{2} n - l \), where \( l << \frac{1}{2} n \). For \( r \) odd, \( p = n^2 + l + 1, q = n-l', n', l' \) integer. The even \( r \) states have unperturbed energies \( \frac{1}{2} n^2 + 2l^2 \) and so are nearly ‘degenerate’ to the base energy \( \epsilon_n = \frac{1}{2} n^2 \). In particular, they are closer to \( \epsilon_n \) than to the base energy of the next representation, \( \epsilon_{n+1} \approx \epsilon_n \pm n \). If the perturbation is symmetric under rotation, the next base energies coupled are \( \epsilon_{n \pm 4} \approx \epsilon_n \pm 4n \). There are, however, many unperturbed states with \( p^2 + q^2 \approx \epsilon_n \). For example, \( 7^2 + 49^2 = \epsilon_{70} \).

However, the matrix elements \( H_{pq,p'q'} \) of a smoothly perturbed Hamiltonian, in the unperturbed basis, are small if \( |p-p'| \) or \( |q-q'| \) is large. Thus, an interpretation of our method, which yields the states of Eq. (10), is that we effectively diagonalize the Hamiltonian in a basis restricted to the unperturbed states ‘degenerate’ with \( \epsilon_n \) and close to \( \frac{1}{2} n, \frac{1}{2} n \). This is the case for the UF, and indeed, we achieve agreement between full numerical diagonalization, diagonalization restricted to ‘degenerate’ states, and the procedure using the solution of the differential equation Eq. (3).

FIG. 1. Absolute value of a localized wave function on the unit square. Uniform field, B=25, n=62, m=0.

For the ideal, zero radius ABFL, there are significant deviations from this scenario. Indeed, most matrix elements of the ABFL perturbed Hamiltonian in the unperturbed basis are infinite. However, it is a weak, logarithmic infinity, and our theory seems to capture the main shape of the wave function, although at the relatively low energies, for which numerical results are available, there are significant corrections. We consider these to be diffraction corrections, arising from a characteristic length shorter than the wavelength.

We therefore use a finite radius, \( \rho \), for the flux line. The field inside the flux tube is \( B_0 = \phi/\pi \rho^2 \). The typical angular deflection suffered by a particle traversing this field is \( \partial \theta \sim (\phi/\phi_0)/k \rho \). To avoid diffraction we require \( \partial \theta \) to be small. In the numerical work shown, we take \( \phi/\phi_0 = 0.1 \), and \( \rho = 0.01 \), while \( k \geq 140 \). This hardly changes the effective potential of Eq. (3). An alternative and equivalent condition is to insist that, on the appropriately defined average \( \overline{m} \), the terms in the Hamiltonian
satisfy \( \langle eA/c \rangle^2/2m \ll \langle e\mathbf{p} \cdot \mathbf{A}/mc \rangle \).

Fig. 3 is for the ABFL case, with \( n = 58, m = 0, r = 0 \) and \( a = \frac{1}{3} \). Fig. 3a) shows \( u_0(x) \) and \( u_0(-x-1) \), its extension into \( x < -\frac{1}{2} \), reflected. For these parameters, \( u_0 \) is not extremely localized, and extends significantly outside \( [-\frac{1}{2}, \frac{1}{2}] \). The remaining plots give \( |\psi_m| = |\partial\psi/\partial n| \). Fig. 3b) plots Eq. (10), 3c) is from diagonalization in the limited basis of the ‘degenerate’ states; and 3d) is from numerical diagonalization in the complete unperturbed basis. To give the flavor of the diffraction effects, we show two numerical results for \( |\psi_m| \) for a zero radius flux line obtained by a special numerical method. Fig. 3e) uses the above parameters, and 3f) is for \( n = 70 \).

We finally argue that the (1,1) states dominate the orbital susceptibility in a parameter range appropriate to experiments. The orbital susceptibility \( \chi \) of a system of noninteracting spinless electrons is given by \( \chi = \partial M/\partial B \) where the magnetization \( M = -\partial\Omega(T, \mu, B)/\partial B \) is that of the grand canonical ensemble,

\[
M(T, \mu, B) = \sum_{n,m} \frac{\partial E_{n,m}}{\partial B} f_D(E_{n,m}(B)). \tag{12}
\]

where \( f_D \) is the Fermi-Dirac distribution function. [The canonical ensemble is required in averaging over many such billiards, but for a single billiard the grand canonical suffices.] The chemical potential \( \mu = k_B T \) is nearly independent of \( B \), since the many states not depending much on field act as a heat bath.

It is easiest, no doubt, to estimate Eq. (12) using the perturbed Berry-Tabor trace formula. \( \Psi \) is equivalent to keeping the \((1, \pm 1)\) periodic orbits and their repetitions in the trace formula. Using the Poisson sum formula, replace the sum on \( n \) in Eq. (12) by an integral over \( k \), and do the integral to obtain

\[
M = \sum_{r,m,s=0}^{\infty} \frac{2\alpha_m L_0}{\pi k_F} \exp \left(-\frac{\omega_r s L}{2k_F}\right) \sin(L_0(k_F - E_m/k_F)). \tag{13}
\]

Here, \( \omega_r = \pi (2r + 1) k_B T \) and \( \alpha_m = \partial E_m/\partial B \). As an example, take \( k_B T \) ten times the level spacing \( d^{-1} \) of all levels, i.e. \( k_B T = 40\pi \). Then, \( \omega_0 L/2 \approx 560 \). If \( k_F \approx 500 \), so that the square contains about 4000 electrons, the exponential suppression will not be too serious for \( r = 0, s = 1 \). Doing the \( m \) sum is possible but harder.

Eq. (13) is obtained from explicit energy levels rather than the action of periodic orbits as found from the trace formula, but the result is the same. Integrable systems have regularities in their energy levels which lead to larger effects in quantities like \( M \) as compared with chaotic systems. For the square, the \((1,1)\) states have the smallest \( L \) and also the largest \( \alpha_m \). The \((2,1)\) resonance does not couple to a constant field. The \((3,1)\) resonances have length \( L_{31} = 2\sqrt{10} = \sqrt{5} L_{11} \) and a potential \( V_{31}(x) = V_{11}(x)/\sqrt{5} \). An interesting case is the \((1,0)\) resonance which has \( L_{10} = 2 \), but this resonance corresponds to classical orbits enclosing no flux. At stronger fields, the curvature of the orbits must be allowed for, and eventually this resonance dominates.

At very strong fields, such that \( R_c < L \), the standard de Haas-van Alphen susceptibility is recovered.

![FIG. 2. Current density of the wave function shown in Fig. 1. The stream lines are plotted, their density proportional to the current density. The sense of the current is paramagnetic.](image)

![FIG. 3. ABFL case. a)-f) \( u_0 \), and b)-f) \( |\partial\psi/\partial n| \), as a function of \( x \), for several cases described in the text.]
1 L. P. Lévy, D. H. Reich, L. Pfeiffer, and K. West, Physica B 189, 204 (1993).
2 D. Ullmo, K. Richter, and R. A. Jalabert, Phys. Reports 276, 1 (1996); K. Richter, Habilitationsschrift (1997); M. Brack and R. K. Bhaduri, *Semiclassical Physics* (Addison-Wesley, Reading, 1997).
3 Y. Aharonov and D. Bohm, Phys. Rev. 115, 485 (1959).
4 M. V. Berry, R. G. Chambers, M. D. Large, C. Upstill, and J. C. Walmsley, Eur. J. Phys. 1, 154 (1980).
5 R. B. Laughlin, Phys. Rev. B 23, 5632 (1981).
6 M. V. Berry and M. Robnik, J. Phys. A 19, 649 (1986); M. V. Berry and M. Robnik, J. Phys. A 19, 669 (1986).
7 G. Date, S. R. Jain, and M. V. N. Murthy, Phys. Rev. E 51, 198 (1996); M. A. M. de Aguiar, Phys. Rev. E 53, 4555 (1996).
8 N. Berglund and H. Kunz, J. Stat. Phys. 83, 81 (1996).
9 P. W. Anderson, Phys. Rev. 109, 1492 (1958).
10 R. E. Prange, R. Narevich, and Oleg Zaitsev, Phys. Rev. E 59, 1694 (1999).
11 E. B. Bogomolny, Nonlinearity 5, 805 (1992).
12 R. E. Prange, R. Narevich, and Oleg Zaitsev, to be published.