Aharonov-Bohm flux and statistics of energy levels in metals

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The statistics of levels in a metallic ring presents a transition from the Gaussian orthogonal ensemble to the Gaussian unitary ensemble, when it is pierced by a magnetic flux ϕ. This transition is driven by the dimensionless parameter $\sqrt{E_c}\varphi$, where E_c is the Thouless energy expressed in units of the interlevel distance and φ is the reduced flux $\varphi=2\pi\phi/\phi_0$. It is very well described by a $E_c\times E_c$ random matrix $\mathcal{H}=\mathcal{H}(S)+i\varphi\mathcal{H}(A)$, where $\mathcal{H}(S)$ and $\mathcal{H}(A)$ are symmetric and antisymmetric matrices whose elements have variance $\sqrt{E_c}$.

I. INTRODUCTION

Electronic disordered systems are characterized by spectra with universal behavior. The statistics of energy levels in complicated systems have been initially studied by Wigner, Dyson, Mehta, and others, to describe the spectra of nuclei.[1–3] These authors describe the properties of a matrix Hamiltonian, with random elements which fluctuate around zero with a Gaussian distribution. Since this random matrix theory (RMT) is independent of any specified microscopic model, it is thought to apply to a variety of very different physical situations, for example, to describe as well nuclear, atomic, or molecular spectra.[4,5] It has been also used in "simple" models of chaos like billiards to understand how the complexity is generated and to describe how the nature of spectrum in quantum mechanics is related to the associated classical problem.[1–5]

The relevance of these ideas to describe the spectrum of small metallic particles was first pointed out by Gorkov and Eliashberg.[6] Later, starting from a microscopic model of disorder and using a supersymmetry formalism and the nonlinear σ model, Efetov could derive the correlation function of the energy levels and show that they are identical to the correlation functions derived from the RMT.[7] A remarkable feature of the RMT is that the distribution of levels only depends on the symmetry properties of the Hamiltonian. If there is time-reversal symmetry, the matrix Hamiltonian has real symmetric elements. The corresponding statistical ensemble is called the Gaussian orthogonal ensemble (GOE) because it is invariant under every orthogonal transformation. The statistics of the levels can be characterized in particular by the following.

(1) The spacing distribution between consecutive levels which is very well described by the Wigner surmise,[1] found for a 2×2 random matrix

$$p(s)=\frac{\pi}{2}s\exp\left[-\frac{\pi}{4}s^2\right], \tag{1.1}$$

where s is the distance between levels in units of the average interlevel distance. The fact that $p(s)\to0$ when $s\to0$ expresses the well-known repulsion between levels. Sivan and Imry found that this repulsion law is observed in the Anderson disordered tight-binding model.[8]

(2) The fluctuation of the number of levels $N(E)$ in a strip of width E which measures the rigidity of the spectrum. It varies as[3]

$$\Sigma_0^2(E)=\langle N^2\rangle-\langle N\rangle^2\approx\frac{2}{\pi^2}\left[\ln(2\pi E)-\frac{\pi^2}{8}+\gamma+1\right], \quad E\geq1, \tag{1.2}$$

where E is in units of the average interlevel distance η. (In this paper, we will set $\eta=1$, most of the time.) γ is the Euler constant. For disordered conductors, this rigidity in the spectrum is at the origin of the universal conductance fluctuations.[9]

When time-reversal symmetry is broken, in a presence of a magnetic field, for example, the Hamiltonian matrix is now complex Hermitian. The statistical ensemble is invariant under unitary transformations and is called Gaussian unitary ensemble (GUE). Realizations of this statistical ensemble have been studied mainly in quantum billiards. The main effect of a non-time-reversal invariance is that the spectrum becomes more rigid. The short-distance repulsion is stronger. It is now characterized by a quadratic (instead of linear) behavior. More precisely

$$p(s)=\frac{32}{\pi^2}s^2\exp\left[-\frac{4}{\pi}s^2\right]. \tag{1.3}$$

The fluctuations of the number of levels is also reduced, roughly by a factor of 2:

$$\Sigma_u^2(E)\approx\frac{1}{\pi^2}[\ln(2\pi E)+\gamma+1], \quad E\geq1. \tag{1.4}$$

The transition between these two ensembles in the random matrix theory has been solved by Pandey and Mehta.[10] They studied the statistics of the eigenvalues of an $N\times N$ matrix Hamiltonian of the form

$$\mathcal{H}=\mathcal{H}(S)+i\alpha\mathcal{H}(A). \tag{1.5}$$

$\mathcal{H}(S)$ is a real symmetric matrix and $\mathcal{H}(A)$ is a real antisymmetric matrix, α is a parameter which interpolates between the two ensembles. $\alpha=0$ describes the GOE statistics and $\alpha=1$ describes he GUE statistics. The purpose of this work in the context of nuclear physics was to detect possible time-reversal symmetry breakdown in nuclear forces.

It has also been noticed that a magnetic flux can change the symmetry of the Hamiltonian, and this effect has been studied in the case of a quantum billiard pierced by a magnetic flux line.[11] Remarkable in this case is that the classical motion is not altered by the flux while the energy levels are.

In this paper, we study the transition between the two ensembles in a metallic system in a magnetic flux. Consider a metallic loop pierced by a magnetic flux. It has been predicted a long time ago and found experimentally very recently that a persistent current is induced by the magnetic flux ϕ.[12,13] The current measures the sensitivity of the spectrum to the magnetic flux:[12]

$$I=-\frac{\partial E_T}{\partial \phi} , \tag{1.6}$$

where E_T is the total energy. It is well known that, using a gauge transformation, the spectrum of the electrons in such a ring is identical to the spectrum of electrons in zero flux, with a change in the boundary conditions. Instead of having periodic-boundary conditions, the wave function obeys $\Psi(x+L)=\Psi(x)e^{2i\pi\phi/\phi_0}$, where L is the perimeter of the ring, ϕ the magnetic flux, and ϕ_0 the flux quantum h/e. As a consequence, the persistent current directly measures the sensitivity of the spectrum to the boundary conditions.[14]

This sensitivity has been emphasized by Thouless who showed that the conductance is a measure of the sensitivity to the boundary conditions:[15]

$$g=\frac{E_c}{\eta} . \tag{1.7}$$

g is the dimensionless conductance, η is the mean interlevel spacing, and the "Thouless energy" E_c is the typical curvature of the levels

$$E_c=\left[\left\langle\left[\frac{\partial^2 e_n}{\partial\varphi^2}\right]^2\right\rangle\Bigg|_{\varphi\to 0}\right]^{1/2} . \tag{1.8}$$

From the Einstein relation, E_c is related to the diffusion coefficient $E_c=D/L^2$. As we will see later, this quantity also measures the correlation between levels.[9]

Our goal in this paper is to describe the crossover between the two statistics induced by a magnetic flux. More precisely, one wants to know how the interpolating parameter α of the random matrix theory is related to the reduced magnetic flux $\varphi=2\pi\phi/\phi_0$. From Thouless, one knows that at small flux, the energy of a level typically varies as $\delta E\approx E_c\varphi^2$. When this excursion becomes of the order of the interlevel distance, we expect a qualitatively different spectrum so that the relevant parameter to describe the transition from GOE to GUE should be proportional to $E_c\varphi^2$. The crossover is thus expected to occur when $\varphi\approx 1/\sqrt{E_c}$.

II. METALLIC RING AND RANDOM MATRIX THEORY

The fluctuations in the spectrum can be characterized by the density-density correlation function, for two energies x and y:

$$K(x,y)=K(x-y)=K(r)=\langle\rho(x)\rho(y)\rangle-\langle\rho(x)\rangle\langle\rho(y)\rangle . \tag{2.1}$$

This function is related to the probability $R(r)$ of finding two levels distant of r:[4]

$$K(r)=\rho_0^2[\delta(r)-1+R(r)] . \tag{2.2}$$

ρ_0 is the average density of states. In principle all higher-order correlation functions could totally characterize the spectrum, but we will use only this one. From this function, one can derive the variance $\Sigma^2(E)$ of the number of levels in a slab of width E, as defined in the Introduction. It can be easily shown that

$$\begin{aligned}\Sigma^2(E)&=\int_0^E\int_0^E K(x,y)dx\,dy\\&=2\int_0^E(E-s)K(s)ds\\&=E-E^2+2\int_0^E(E-s)R(s)ds .\end{aligned} \tag{2.3}$$

The function R has been calculated by Efetov for a microscopic model of disorder.[7] In the orthogonal and unitary ensembles, this function is

$$R_u(r)=1-\frac{\sin^2 x}{x^2} , \tag{2.4}$$

$$R_o(r)=1-\frac{\sin^2 x}{x^2}-\frac{d}{dx}\left[\frac{\sin x}{x}\right]\int_1^\infty\frac{\sin xt}{t}dt , \tag{2.5}$$

with $x=\pi r$. The spectral rigidity is derived from the integration [Eq. (2.2)] (Refs. 3 and 4)

$$\Sigma_u^2(E)=\frac{1}{\pi^2}[\ln(2\pi E)+\gamma+1-\cos(2\pi E)-\mathrm{Ci}(2\pi E)]+E\left[1-\frac{2}{\pi}\mathrm{Si}(2\pi E)\right] , \tag{2.6}$$

$$\Sigma_0^2(E)=2\Sigma_u^2(E)+\left[\frac{\mathrm{Si}(\pi E)}{\pi}\right]^2-\frac{\mathrm{Si}(\pi E)}{\pi} . \tag{2.7}$$

These results *exactly coincide* with the expressions obtained from the random matrix theory.[3,16] $R(r)$ and $\Sigma^2(E)$ have been calculated for the two limits and in principle could be also known in the cross-over regime. This crossover is more easily seen in the formulation of Al'tshuler and Shklovskii of the fluctuation of energy levels.[9] The correlation function $K(r)$ can be calculated from microscopic theory, using a diagrammatic technique where only a class of diagrams is kept. They get

$$K(r)\approx-\frac{\rho_0^2}{2\pi^2}\mathrm{Re}\sum_{\substack{q_\alpha\\ \alpha=D,C}}\frac{1}{(r+i\delta+iDq_\alpha^2)^2} . \tag{2.8}$$

δ is a cutoff which originates, for example, from inelastic collisions. In the absence of such processes, and *in a* *closed system,* it is taken of the order of the interlevel distance. The sum over α corresponds to the diffusion propagator (so-called diffuson) and particle-particle propagator (so-called cooperon) diagrams. The wave vectors q_α are quantized by the boundary condition $q_\alpha^x = 2\pi n_x/L_x$, $n_x \in \mathbb{Z}$, along the direction x of the ring, and $q_\alpha^\mu = \pi n_\mu / L_\mu, n_\mu \in \mathbb{N}$, along the transverse directions. When $r < E_c = D/L^2$, the correlation function is

$$K(r) \approx -\frac{\rho_0^2}{\pi^2}\mathrm{Re}\frac{1}{(r+i\delta)^2} . \tag{2.9}$$

This form of the correlation function leads to

$$\Sigma_0^2(E) \approx \frac{1}{\pi^2}\ln\frac{E^2+\delta^2}{\delta^2} , \quad 1 \le E \le E_c . \tag{2.10}$$

This expression approximates the result of Efetov [Eq. (2.7)] and has asymptotically the same behavior. In the presence of a magnetic flux, the boundary conditions are changed. The momentum of the diffuson is still the same but the cooperon propagator momentum along the direction of the ring gets a shift proportional to the flux $q_c^x = (2\pi n_x/L_x) + (4\pi/L_x)(\phi/\phi_0) = (1/L_x)(2n_x\pi + 2\varphi)$. The factor 2 in front of φ comes from the fact that q is the momentum of a pair of particles. In a flux, the correlation function thus becomes[17,18]

$$K(r,\varphi) = -\frac{\rho_0^2}{2\pi^2}\mathrm{Re}\left[\frac{1}{(r+i\delta)^2} + \frac{1}{(r+i\delta+4E_c\varphi^2)^2}\right] . \tag{2.11}$$

One can now derive the spectral rigidity, when $E \le E_c$:

$$\Sigma^2(E,\varphi) \approx \frac{1}{2\pi^2}\left[\ln\left[1+\frac{E^2}{\delta^2}\right] + \ln\left[1+\frac{E^2}{(\delta+4E_c\varphi^2)^2}\right]\right] ,$$
$$1 \le E \le E_c . \tag{2.12}$$

When φ is large, the second term vanishes so that the spectral rigidity is roughly divided by a factor 2, as we expect from the more sophisticated calculation.[7]

On the other hand, the crossover between GOE and GUE ensembles has been completely solved in the RMT by Pandey and Mehta.[10] Starting from the $N \times N$ matrix Hamiltonian (1.5), they introduce the parameter λ as (for small α):

$$\lambda = \frac{\alpha\sqrt{N}}{\pi} \tag{2.13}$$

which expresses the variance of the imaginary part of the matrix elements in units of the average spacing. (In the RMT, the average spacing actually depends on the position in the band since the density of states is a semicircle.) In terms of this parameter, the function $R(r)$ has been calculated exactly:

$$R(r) = 1 - \left[\frac{\sin\pi r}{\pi r}\right]^2 + \frac{1}{\pi^2}\int_0^\pi dk\, k\sin(kr)\exp(2\lambda^2k^2)\int_\pi^\infty dt\frac{\sin(tr)}{t}\exp(-2\lambda^2t^2) . \tag{2.14}$$

This expression differs from Eqs. (2.4) and (2.5) for $R_u(r)$ and $R_o(r)$, only by the two exponential factors. $R(r) \to R_o(r)$ when $\lambda \to 0$ and $R(r) \to R_u(r)$ when $\lambda \to \infty$.

Again, one can deduce the spectral rigidity $\Sigma^2(E,\lambda)$ from the integration of $R(r,\lambda)$. An extremely good approximation of the result can be written as[19]

$$\Sigma^2(E,\lambda) \approx E_u^2(E) + \ln\left[1+\frac{E^2}{(2\tau/\pi+4\pi\lambda^2)^2}\right] \tag{2.15}$$

with $\tau \approx 0.615$. Expressions (2.12) and (2.15), respectively, deduced from the microscopic theory and RMT are very similar. This suggests the following correspondence between the parameters of the RMT and the microscopic model:

$$\delta = \frac{2\tau}{\pi} , \tag{2.16a}$$

$$4\pi\lambda^2 = 4E_c\varphi^2 . \tag{2.16b}$$

Equation (2.16a) shows that the cutoff δ of the perturbation calculation is of the order of the interlevel distance.

III. NUMERICAL RESULTS

We have studied the statistics of levels numerically within the Anderson model. The transfer term is taken as a constant t between first neighbors. The field effect is simply to change the boundary condition along the ring so that the transfer term gets a phase factor $\exp(2i\pi\phi/\phi_0)$ after one loop along the ring. Open boundary conditions are taken in the two other directions. The disorder is given by a random choice of the on-site energy between $-W/2$ and $W/2$. This model has been used recently to calculate numerically the amplitude of the persistent currents.[20] Here, we show results for a $64 \times 14 \times 14$ sample. We have chosen values of W so that the system is metallic. The crossover to localized and ballistic regimes will be described in a forthcoming paper. The transition-metal insulator in zero field has already been described by Al'tshuler *et al.*[21] We have calculated $\Sigma^2(E) = \langle N(E,\varepsilon)^2\rangle_\varepsilon - \langle N(E,\varepsilon)\rangle_\varepsilon^2$ where $\langle\ \rangle_\varepsilon$ is the average on disorder. The ergodic hypothesis asserts that this quantity is equal to the *ensemble* average done at fixed ε.[22] This hypothesis certainly holds for $E \le E_c$ and becomes wrong when $E \ge E_c$. It is also known that when $E \ge E_c$, the spectrum loses its rigidity[9]

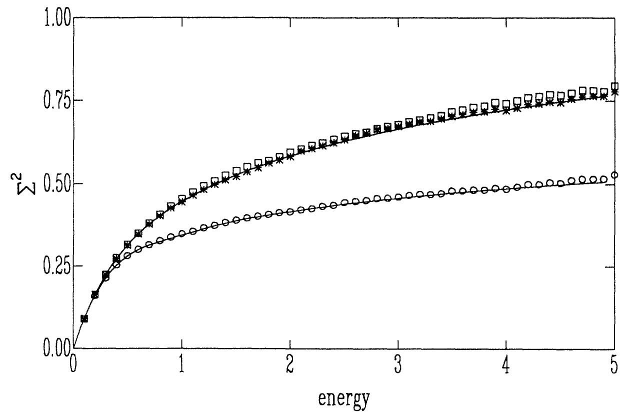

FIG. 1. $\Sigma^2(E,\phi)$ for three values of the magnetic flux. Squares, $\varphi=0$; circles, $\varphi=\pi/2$; stars, $\varphi=\pi$. Here $W/t=1.5$. The two solid lines are the RMT results for the orthogonal (top line) and unitary (bottom line) ensembles, given by Eqs. (2.6) and (2.7).

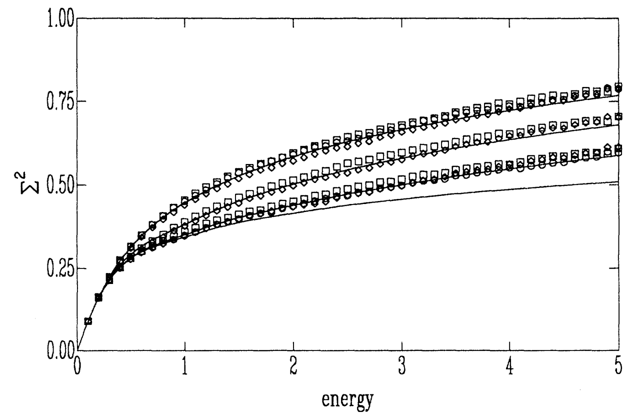

FIG. 3. $\Sigma^2(E,\phi)$ for increasing values of the flux in the cross-over region, for three values of the disorder W. Squares, $W=1.5$, $\varphi=0$, $\varphi=\pi/20$, and $\varphi=\pi/10$; circles, $W=2$, $\varphi=0$, and $\varphi=3\pi/20$; triangles, $W=3$, $\varphi=0$, $\varphi=\pi/10$, and $\varphi=\pi/5$. These three series look exactly the same, provided φ/W has been kept constant. This shows that the transition is driven by the parameter $\sqrt{E_c}\varphi$.

so that it cannot be described by the RMT. For these reasons, we limit our numerical investigation to $E \le E_c$. Figure 1 shows the quantity $\Sigma^2(E)$ for three values of the magnetic flux: $0, \phi_0/4$, and $\phi_0/2$. It is seen that for $\phi=0$ and $\phi_0/2$, the fluctuations are very well described by the orthogonal ensemble while for $\phi=\phi_0/4$, it is clearly fitted by the unitary case. The half-quantum case has no time-reversal symmetry breaking since the phase factors in the Hamiltonian become real (-1) for this flux. This situation is named by Berry and Robnick as "false T breaking."[11]

Then we have studied the crossover between GOE and GUE by varying the magnetic flux. Figure 2 shows the fluctuations for increasing values of the flux. In this case where $W/t=2$, the curves for finite ϕ are very well fitted by the RMT, if one chooses $\varphi \approx 2\pi\lambda/5.6$ which implies $E_c \approx 8/\pi$. Since one knows that E_c varies like $1/W^2$, one can deduce the relationship between the flux and the coefficient λ of the RMT:

$$\lambda = \left[\frac{E_c}{\pi}\right]^{1/2} \varphi \approx \frac{11.2}{W}\frac{\varphi}{2\pi} . \tag{3.1}$$

We have checked this E_c dependence of λ. Figure 3 shows $\Sigma^2(E,\varphi)$ versus E for various values of the disorder, $W/t=1.5$, 2, and 3, so that φ/W is kept constant. The fact that we get a universal behavior proves that the transition GOE-GUE is governed by the unique parameter $\sqrt{E_c}\varphi$. In Fig. 4, we have plotted $\Sigma^2(E,\varphi)$ versus φ for constant E. We see that the transition is completed when $\varphi \approx 1/\sqrt{E_c}$ and that for higher flux the statistics remain GUE until the vicinity of the half-flux quantum is reached.

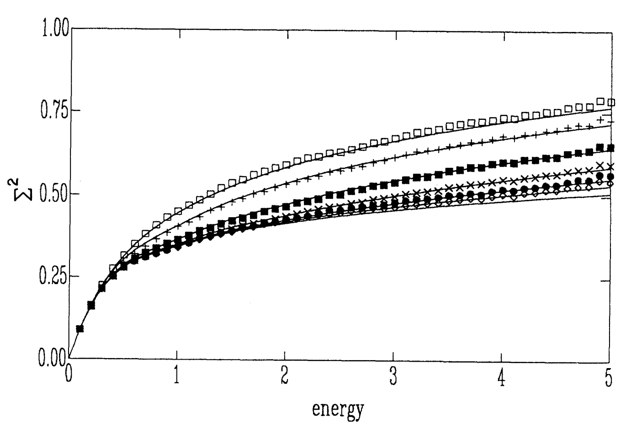

FIG. 2. $\Sigma^2(E,\phi)$ for increasing values of the flux in the cross-over region. Squares, $\varphi=0$; pluses, $\varphi=\pi/20$; solid squares, $\varphi=\pi/10$; crosses, $\varphi=3\pi/20$; solid circles, $\varphi=\pi/5$. These curves are very well fitted by the RMT crossover curves with a parameter $\lambda=5.6\varphi/2\pi$. Here $W/t=2$.

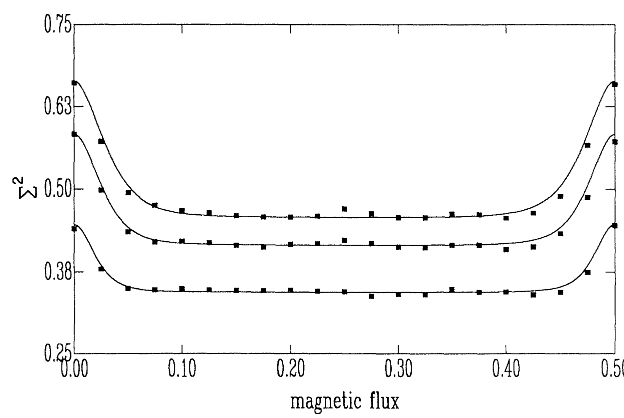

FIG. 4. $\Sigma^2(E,\phi)$ vs ϕ at constant E. The transition GOE-GUE is completed when $\varphi/2\pi \approx 0.05$, i.e., from Eq. (3.1), $\lambda \approx 0.4$.

Figure 5 shows the distribution function $p(s)$ of the spacing s between nearest levels and its integral $\int_0^s p(u)du$. The excellent agreement with the RMT prediction is seen more easily on the integrated distribution function (5b). In zero flux, or when $\phi=\phi_0/2$, it follows the GOE Wigner surmise [Eq. (1.1)], as found already in Ref. 8 for $\phi=0$. When $\phi=\phi_0/4$, the distribution follows the GUE behavior with a quadratic departure at the origin [Eq. (1.3)]. When the flux increases from zero, the distribution progressively shifts from the GOE behavior. The crossover to a finite value of the parameter λ has been calculated in the literature only for a 2×2 matrix for which we know that, in the two limits, the calculated $p(s)$ is a very good approximation of the distribution in large size matrices.[4,19] In between the distribution is[19]

$$p(s,\alpha)=\frac{s}{4v^2\sqrt{1-\alpha^2}}\exp\left[\frac{-s^2}{8v^2}\right]\operatorname{erf}\left[\left[\frac{1-\alpha^2}{8\alpha^2v^2}\right]^{1/2}s\right]. \tag{3.2}$$

By connecting the values of $\lambda_2(\alpha)$ for this 2×2 matrix[19]

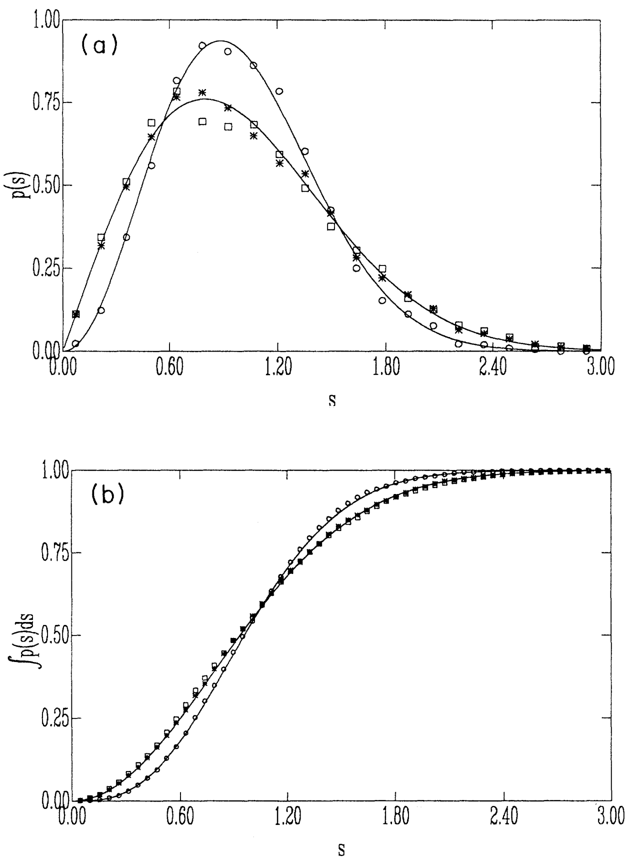

FIG. 5. (a) $p(s,\phi)$ for extreme values of the flux so that the distribution is GOE (squares, $\varphi=0$; stars, $\varphi=\pi$) or GUE (circles, $\varphi=\pi/2$). The solid lines are the Wigner surmises. Here $W=2$. (b) $\int_0^s p(r,\phi)dr$, for the same values of flux and disorder. The curves are the RMT result. They start as $s^{\beta+1}$, with $\beta=1$ for the GOE and $\beta=2$ for the GUE.

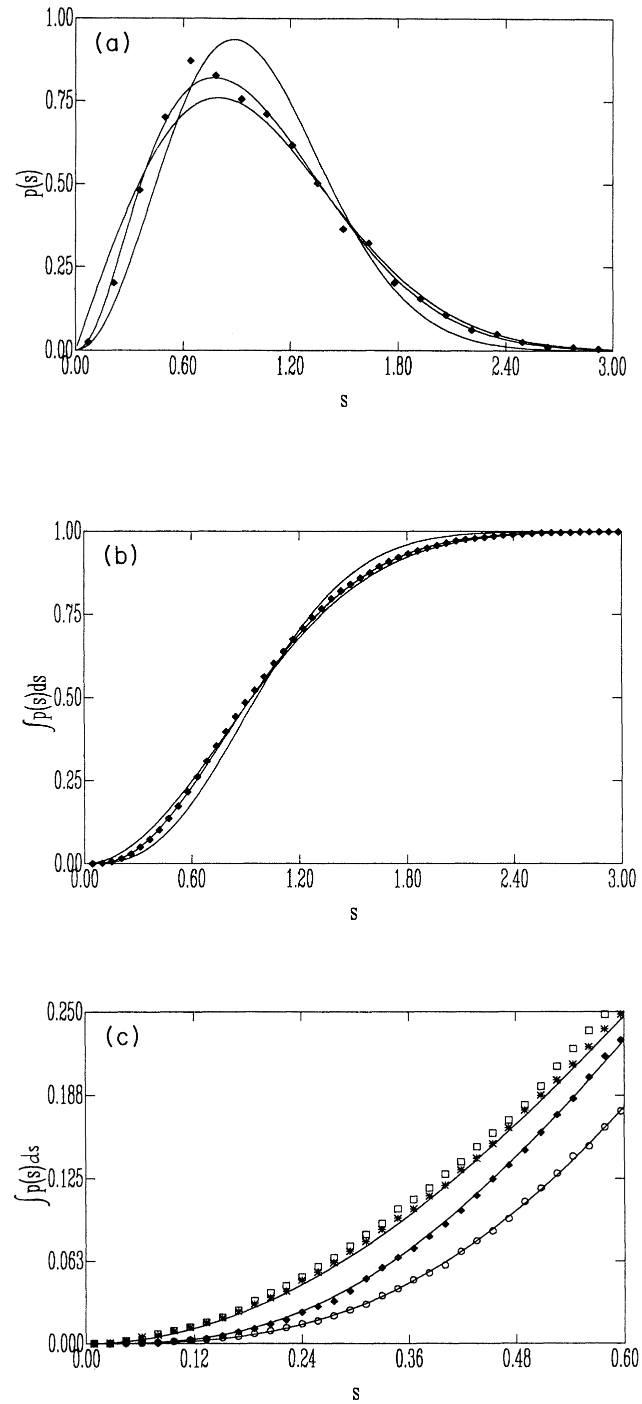

FIG. 6. (a) $p(s,\phi)$ for $\varphi=\pi/20$. Two of the solid lines show the extreme behaviors corresponding to the orthogonal and unitary ensembles and the intermediate one is the analytical result of the RMT of a 2×2 matrix for $\alpha=0.31$ [instead of $\alpha=0.37$ that we would expect from $\lambda_2(\alpha)=\lambda(\varphi)$]. (b) $\int_0^s p(r,\phi)dr$, for the same values of the flux and disorder. (c) $\int_0^s p(r,\phi)dr$, for the same values of flux and disorder, at small separation s. It is seen that, as soon as λ is nonzero, the distribution deviates from GOE and follows the GUE behavior in s^3. Then it comes closer to the GOE behavior.

$$\lambda_2 = \alpha v/d = \alpha \left[\frac{\pi}{8}\right]^{1/2} \left[(1-\alpha^2)^{-1/2}\arctan\left[\frac{(1-\alpha^2)^{1/2}}{\alpha}\right] + \alpha\right]^{-1} \tag{3.3}$$

to the $\lambda(\varphi)$ of our physical problem $\lambda = \sqrt{E_c/\pi}\varphi$, one deduces the correspondence between φ and $\alpha(\varphi)$ and then the distribution $p(s,\alpha) = p(s, \sqrt{E_c}\varphi)$. Figure 6 shows that the numerical $p(s)$ in a finite flux is very well fitted by the function $p(s,\alpha)$ of RMT [but the value of α is slightly different from the one deduced from the condition $\lambda_2(\alpha) = \lambda(\varphi)$, Fig. 6]. It is also seen that for small s, the distribution behaves as the GUE as soon as λ is finite.

IV. CONCLUSION

We have shown that the statistics of levels in a metallic ring pierced by a magnetic flux presents a transition from GOE to GUE. This transition is characterized by the dimensionless parameter $\sqrt{E_c}\varphi$. The transition can be described by a random $N \times N$ matrix $\mathcal{H} = \mathcal{H}(S) + i\alpha\mathcal{H}(A)$. Since the physical spectrum to be described loses its rigidity on an energy range wider than E_c, the size N of the random matrix has to be proportional to E_c/η. The variance v^2 of the matrix elements is proportional to ηE_c (so that the interlevel distance η is independent of E_c). α is proportional to the dimensionless magnetic flux φ. The mapping between the parameters of the RMT and of the metallic ring is

$$\alpha \propto \varphi ,$$

$$v \propto \sqrt{E_c} ,$$

$$N \propto E_c ,$$

and the parameter λ which describes the transition is, for small α

$$\lambda = \frac{\alpha v}{\eta} = \varphi \left[\frac{E_c}{\pi}\right]^{1/2}$$

as found from Eq. (2.16). The transition is completed when $\lambda \approx 1$, i.e., when the typical shift of a level is of the order of the average spacing.[23] This happens when $\sqrt{E_c}\varphi \approx \eta$.

When α increases, the variance v^2 must be divided by $1+\alpha^2$ to keep the average interlevel distance fixed. Thus the random matrix must have the form

$$\mathcal{H} = \frac{1}{\sqrt{1+\alpha^2}}[\mathcal{H}(S) + i\alpha\mathcal{H}(A)] .$$

Since the spectrum is periodic with period ϕ_0 and since it has GOE statistics around $\phi = n\phi_0/2$, we conjecture that, for larger flux, the parameter α which describes the statistics of levels is $\alpha = tg\varphi$, so that $\lambda = (E_c/\pi)^{1/2}\sin\varphi$ and

$$\mathcal{H} = \cos\varphi\mathcal{H}(S) + i\sin\varphi\mathcal{H}(A) .$$

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