ORBITAL MAGNETISM IN QUANTUM DOTS: A SEMICLASSICAL APPROACH

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In this communication we review our recent work[1),2)] on the magnetic response of ballistic microstructures. The study of orbital magnetism in an electron gas has a long history, and was initiated by Landau[3)] only four years after the discovery of the Schrödinger equation. For a free electron gas the low-field susceptibility is diamagnetic. In three and two dimensions it attains, respectively, the values $\chi_L^{3D} = -(1/12\pi^2)e^2k_F/mc^2$ and $\chi_L^{2D} = -(1/12\pi)e^2/mc^2$, where k_F is the Fermi wavevector. The modifications of these results arising from constraining the electron gas in a finite volume have been the object of several studies[4)]. On the other hand, in the last few years the field known as Quantum Chaos has been dealing with questions regarding the differences at the quantum level between systems whose underlying classical mechanics is chaotic and those where it is regular. Nakamura and Thomas[5)] were the first to address the problem of orbital magnetism from a Quantum Chaos point of view by numerically studying the differences in the magnetic response of circular and elliptic billiards.

The interest on the orbital magnetism of confined systems, and its connection with Quantum Chaos has recently been renewed with the experimental realization of ballistic quantum dots lithographically defined on high mobility semiconductor heterojunctions. Experiments by Lévy *et al* [6)] yielded, for an ensemble of 10^5 microscopic ballistic squares[7)], a paramagnetic low-field susceptibility being more than an order of magnitude larger than $|\chi_L^{2D}|$. Combining a thermodynamic formalism that closely follows that developed in the context of persistent currents with a semiclassical approach, we are able to show that *the enhancement of the low-field susceptibility with respect to the Landau value is due to large modulations in the density of states caused by families of periodic orbits* present in integrable systems.

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The magnetic susceptibility of a two-dimensional system of N electrons occupying an area A is given by the change of the free energy F under the effect of a magnetic field,

$$\chi = -\frac{1}{A}\left(\frac{\partial^2 F}{\partial H^2}\right)_{N,T} . \tag{1}$$

In the macroscopic limit of very large N and A the choice of the ensemble is a matter of convenience, we can equally well work in the grand canonical ensemble (GCE) at fixed chemical potential and obtain the susceptibility as a derivative of the thermodynamical potential Ω,

$$\Omega(T,\mu,H) = F(T,N,H) - \mu N = -\frac{1}{\beta}\int \mathrm{d}E\ \rho(E,H)\ \ln\left(1+\exp\left[\beta(\mu-E)\right]\right) . \tag{2}$$

$\rho(E,H)$ is the density of states and $\beta = 1/k_B T$. The above mentioned equivalence between the ensembles breaks down in the mesoscopic regime of small structures[8], and therefore it is important to work with the canonical expression (1). Separating ρ into a mean part ρ^0 (that scales as the area of the system) and an oscillatory component ρ^{osc} (that in a semiclassical approach is given by the sum over periodic trajectories), we define a mean chemical potential μ^0 from $N = \int \mathrm{d}E \rho(E) f(E-\mu) = \int \mathrm{d}E \rho^0(E) f(E-\mu^0)$. ($f$ is the Fermi-Dirac distribution function.) Since ρ^0 and ρ^{osc} have different order in the semiclassical parameter $\hbar$, we can expand the terms in Eq. (2) up to second order in $\rho^{\mathrm{osc}}/\rho^0$ obtaining[9]

$$F(N) \simeq F^0 + \Delta F^{(1)} + \Delta F^{(2)} , \qquad F^0 = \mu^0 N + \Omega^0(\mu^0) , \tag{3}$$

$$\Delta F^{(1)} = \Omega^{\mathrm{osc}}(\mu^0) , \qquad \Delta F^{(2)} = \frac{1}{2\rho^0(\mu^0)}\left[\int \mathrm{d}E\ \rho^{\mathrm{osc}}(E)\ f(E-\mu^0)\right]^2 . \tag{4}$$

Ω^0 and Ω^{osc} are defined by using respectively ρ^0 and ρ^{osc} instead of ρ in Eq. (2). F^0 is field independent to leading order in a semiclassical expansion. Higher order terms in $\hbar$ give rise to the standard two-dimensional diamagnetic Landau susceptibility χ_L^{2D} *regardless of the confining potential* [2]. The decomposition (3)-(4) has the advantage of that the corrections $\Delta F^{(1)}$ and $\Delta F^{(2)}$ are expressed as simple functions of the oscillatory part of the density of states which can be evaluated semiclassically.

In order to calculate the oscillating part of the density of states we use a semiclassical approach starting from the expression of ρ^{osc} in terms of the trace of the semiclassical Green function[10],

$$G_E^{\mathrm{sc}}(\mathbf{r}',\mathbf{r}) = \sum_t D_t \exp\left[i\left(\frac{S_t}{\hbar} - \left(\eta_t - \frac{1}{2}\right)\frac{\pi}{2}\right)\right] . \tag{5}$$

The sum runs over all classical trajectories t joining $\mathbf{r}$ to $\mathbf{r}'$ at energy E. S_t is the action integral along the trajectory. For billiards without magnetic field we simply have $S_t/\hbar = kL_t$ where $k = \sqrt{2mE}/\hbar$ and L_t is the length of the trajectory. The amplitude D_t takes care of the classical probability conservation and η_t is the Maslov index.

The free energy corrections $\Delta F^{(1)}$ and $\Delta F^{(2)}$ are therefore given as sums over classical trajectories, each term being the convolution in energy of the semiclassical contribution (oscillating as kL_t) with the Fermi factor (smooth on the scale of β^{-1}). This implies that the contribution of a given trajectory to $\Delta F^{(1)}$ at finite temperature is reduced with respect to its $T=0$ counterpart by a multiplicative factor $R(T) = (L_t/L_c)\sinh^{-1}(L_t/L_c)$, with $L_c = \hbar^2 k_F \beta/(\pi m)$. A factor $R^2(T)$ is needed for $\Delta F^{(2)}$. At high temperatures $R(T)$ yields *an exponential suppression of long trajectories*. Therefore the fluctuating part of the free energy, and χ, are dominated by trajectories with $L_t \leq L_c$, which are the only ones considered in our analysis.

The square constitutes the generic case of a regular system: it is integrable at zero magnetic field, but a perturbing field breaks the integrability. This implies that in calculating the susceptibility we cannot use neither the standard Berry-Tabor trace formula[11)] (valid for integrable systems) nor the Gutzwiller trace formula[10)] (applicable when the periodic orbits are well separated). On the other hand, we can directly use Eq. (5) since the simplicity of the geometry allows the enumeration of all closed trajectories and the evaluation of the field dependence of their contribution to $\rho^{\rm osc}$. Given the exponential suppression of long trajectories, the finite-temperature susceptibility will be dominated by the contribution to $\rho^{\rm osc}$ of the family of closed trajectories which, for $H \to 0$, tends to the family of shortest periodic orbits with non-zero enclosed area. We note this family as (1,1) since the trajectories bounce once on each side of the square (upper inset, Fig. 1). Their length is $L_{11} = 2\sqrt{2}a$, which is of the order of the cut off length $L_c \approx 2a$ at the temperature of the experiment of Ref. 6.[12)]

Applying classical perturbation theory for the change in the action S_t of trajectories (1,1) under the effect of a small magnetic field (such that the cyclotron radius r_c verifies $r_c \gg a$), and performing the energy integrations of Eqs. (4) we obtain for the contributions to the susceptibility coming from $\Delta F^{(1)}$ and $\Delta F^{(2)}$ respectively

$$\frac{\chi^{(1)}}{|\chi_L^{2D}|} = \frac{3}{(\sqrt{2}\pi)^{5/2}} (k_F a)^{3/2} \sin\left(k_F L_{11} + \frac{\pi}{4}\right) \frac{\mathrm{d}^2 C}{\mathrm{d}\varphi^2} R(T) , \tag{6}$$

$$\frac{\chi^{(2)}}{|\chi_L^{2D}|} = -\frac{3}{\sqrt{2\pi^3}} k_F a \sin^2\left(k_F L_{11} + \frac{\pi}{4}\right) \frac{\mathrm{d}^2 C^2}{\mathrm{d}\varphi^2} R^2(T) . \tag{7}$$

The field dependence enters through the function

$$\mathcal{C}(\varphi) = \frac{1}{\sqrt{2\varphi}} \left[\cos(\pi\varphi)\, \mathrm{C}(\sqrt{\pi\varphi}) + \sin(\pi\varphi)\, \mathrm{S}(\sqrt{\pi\varphi})\right] . \tag{8}$$

C and S are respectively the cosine and sine Fresnel integrals, and $\varphi = \Phi/\Phi_0$ is the total flux $\Phi = Ha^2$ inside the square measured in units of $\Phi_0 = hc/e$ (the fundamental flux). $\chi^{(1)}$ is the leading contribution to the susceptibility of a given square since its typical magnitude is much larger than $|\chi_L^{2D}|$ and that of $\chi^{(2)}$. On the other hand, $\chi^{(1)}$ can be paramagnetic or diamagnetic (Fig. 1) and it will vanish by averaging over an ensemble of squares where the dispersion of $k_F L_{11}$ is of the order of 2π. Since $\sin^2(k_F L_{11} + \pi/4)$ averages to 1/2, the average susceptibility is given by $\chi^{(2)}$ (solid line, Fig. 2). In particular, the zero-field susceptibility of the ensemble is paramagnetic and has a value $4\sqrt{2}/(5\pi)k_F a R^2(T)$ [13]. For ensembles with a wide distribution of lengths (in the experiment of Ref. 6 the dispersion in size across the array is estimated between 10 and 30%) the dependence of $\mathcal{C}$ on a (through φ) has to be considered. Since the scale of variation of $\mathcal{C}$ with a is much slower than that of $\sin^2(k_F L_{11} + \pi/4)$ we can effectively separate the two averages and obtain the total mean by averaging the local mean. The low-field oscillations of $\langle\chi\rangle$ with respect to φ are suppressed under the second average (performed for a gaussian distribution with a 30% dispersion, dashed line in Fig. 2), while the zero-field behavior remains unchanged.

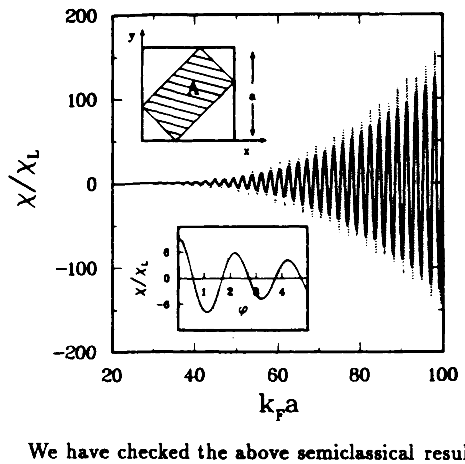

Fig.1: Magnetic susceptibility of a square as a function of $k_F a$ at zero field and a temperature equal to 10 level-spacings from numerical calculations (dotted), and from semiclassical calculations (solid). The period $\pi/\sqrt{2}$ indicates the dominance of the shortest periodic orbits enclosing non-zero area with length $L_{11} = 2\sqrt{2}a$ (upper inset). Lower inset: amplitude of the oscillations (in $k_F L_{11}$) of χ as a function of the flux through the sample from Eq. (6) (solid) and numerics (dashed).

We have checked the above semiclassical results by calculating the partition function $Z = \exp(-\beta F)$ after direct diagonalization of the hamiltonian. As shown in Figs. 1 and 2, the agreement between semiclassical theory and exact quantum mechanical calculations is excellent, demonstrating that the concept of classical trajectories is essential for the physical understanding of the phenomenon and showing the importance of the family (1,1) in the finite-temperature, low-field regime of interest.

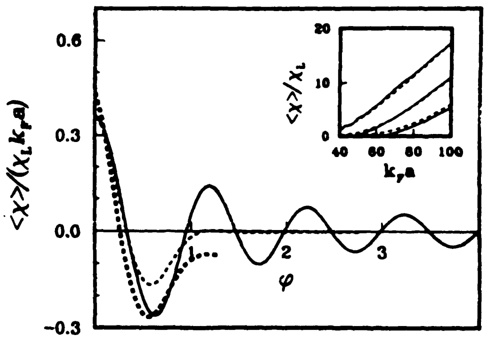

Fig.2: Average magnetic susceptibility for an ensemble of squares with a small dispersion of sizes (solid) and with a large dispersion (dashed) from semiclassical calculations. Thick dashed: average from numerics. The shift of the numerical with respect to the semiclassical results reflects the Landau susceptibility (due to F^0). Inset: average susceptibility as a function of $k_F a$ for various temperatures (4,6 and 10 level spacings) and a flux $\varphi = 0.15$, from semiclassics (solid) and numerics (dashed).

The generic case of an integrable system perturbed by a weak magnetic field can be treated more generally within a semiclassical approach[2], and one obtains the same qualitative behaviour as for the square geometry (Eqs. (6)-(7)). That is, a $(k_F a)^{3/2}$ dependence for the typical value of $\chi^{(1)}$ (which can be diamagnetic or paramagnetic) and $k_F a$ dependence for $\chi^{(2)}$ which gives the average susceptibility of an ensemble. The numerical prefactors obviously depend on the particular geometry in consideration. Circles and rings, for instance, which have the same parametric dependence constitute a particularly simple case since the rotational symmetry avoids that a perturbing magnetic field breaks integrability, and we can calculate the magnetization by a direct application of the Berry-Tabor trace formula. In ring geometries it is customary to measure the magnetic response in terms of the persistent currents, and our semiclassical calculations are in reasonable agreement with the existing experiments in the ballistic regime[14].

For chaotic systems (of typical length a) the Gutzwiller Trace Formula provides the appropriate path to calculate $\rho^{osc}(E, H)$. For temperatures at which only a few short periodic orbits are important, $\chi^{(1)}$ can be paramagnetic or diamagnetic and its typical value is of the order of $k_F a \chi_L^{2D}$ [15]. Extending this analysis to the case of an ensemble of chaotic systems we obtain $\langle\chi\rangle \propto |\chi_L^{2D}|$. The individual χ are larger, by a factor $(k_F a)^{1/2}$ in regular geometries than in chaotic systems. For $\langle\chi\rangle$ the difference is of the order of $k_F a$. These differences are due to the large oscillations of ρ in regular systems induced by families of periodic trajectories. Therefore, the different magnetic response according to the geometry does not arise as a long-time property (linear vs. exponential trajectory divergences) but as a short-time property (family of trajectories vs. isolated trajectories).

It is important to notice that the semiclassical concepts that we have outlined can be extended outside the weak-field regime. For the case of the square[2)] the essential physical behavior can be understood from only one kind of trajectories in each field regime: the family (1,1) for weak fields $r_c \gg a$, the bouncing trajectories of electrons that are reflected between opposite sides of the square for $r_c \approx a$, and the cyclotron orbits that give the standard de Haas - van Alphen oscillations when $r_c < a/2$.

We have so far ignored the possibility of impurity scattering. Our model of a clean system is quite appropriate from a Quantum Chaos point of view and also constitutes a good first order approximation to the physics of quantum dots. In order to get a more realistic description of the actual microstructures we consider the corrections to the above picture due to the presence of weak disorder scattering. Including the effect of the disorder in our semiclassical framework we obtain[2)] the rather natural result that the two contributions to the susceptibility coming from the (1,1) family are reduced with respect to their clean counterparts as $\chi^{(1)} = \chi_{\rm cl}^{(1)} e^{-L_{11}/2l}$ and $\chi^{(2)} = \chi_{\rm cl}^{(2)} e^{-L_{11}/l}$, where l is the elastic mean free path. We have checked these relationships numerically and in Fig. 3 we present the results of the typical susceptibility for δ-function impurities and various l's. We have an excellent agreement with the semiclassical prediction for very weak disorder, while for $l \approx a$ the semiclassical approximation tends to overestimate the reduction. It is important to notice that the long trajectories, very sensitive to the presence of disorder, are completely irrelevant at finite temperatures.

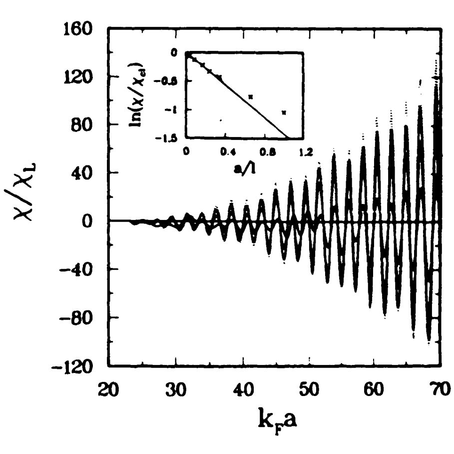

Fig.3: Zero-field susceptibility of a disordered square as a function of $k_F a$ from numerical calculations with $l/a = 12$, 3 and 1 (solid). The temperature is equal to 6 level spacings, the potential scattering is δ-like, and in each case an average over five impurity configurations has been performed. The clean case ($l = \infty$) is shown for comparison (dotted). Inset: logarithm of the reduction factor as a function of the inverse mean free path from numerical calculations (crosses). The straight line is the semiclassical prediction.

Ref. 6 yielded a paramagnetic susceptibility at $H = 0$ with a value of approximately 100 (with an uncertainty of a factor of 4) in units of χ_L. The two electron densities considered in the experiment are 10^{11} and $3 \times 10^{11} cm^{-2}$ corresponding to approximately 10^4 occupied levels per square. For a temperature of $40mK$ Eq. (7) gives, respectively, for the zero-field susceptibility values of 60 and 170. A further reduction arises from the effect of disorder and we are then within the order of magnitude of the experiment (given the experimental uncertainties in the magnitude of the susceptibility and in the determination of the elastic mean free path). The field scale for the decrease of $\langle\chi(\varphi)\rangle$ is of the order of one flux quantum through each square, in reasonable agreement with our theoretical findings. A better knowledge of the actual impurity potential and the inclusion of interaction effects are desirable in order to attempt a more precise comparison with experiment. These more refined theories should necessarily incorporate the simple physics that we have discussed: the enhancement of the weak field susceptibility due to families of short periodic orbits.

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