Orbital Magnetism in Ensembles of Ballistic Billiards

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Abstract

We calculate the magnetic response of ensembles of small two-dimensional structures at finite temperatures. Using semiclassical methods and numerical calculation we demonstrate that only short classical trajectories are relevant. The magnetic susceptibility is enhanced in regular systems, where these trajectories appear in families. For ensembles of squares we obtain a large paramagnetic susceptibility, in good agreement with recent measurements in the ballistic regime.

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A free electron gas at temperature $T$ and magnetic field $H$ such that $k_B T \gg \hbar w (w = eH/mc)$ exhibits a small diamagnetic response \[1\]. This behavior persists when the electrons are placed in periodic or weak-disorder potentials \[2\]. When the system is constrained to a finite volume the confining energy appears as a relevant scale giving rise to finite-size corrections to the Landau susceptibility. These corrections have been the object of several theoretical studies in the last few years for the case of clean \[3,4\] and disordered \[5\] systems, and received renewed interest with recent experiments of Lévy et al. \[6\]: Measurements on an ensemble of $10^5$ microscopic, phase-coherent, ballistic \[7\] squares lithographically defined on a high mobility GaAs heterojunction yielded a large paramagnetic susceptibility at zero field, decreasing on the scale of approximately one flux quantum through each square. These experiments have been important in orienting the theoretical studies towards the physically relevant questions associated with the magnetic response of small systems. In particular, the role of finite temperature and the necessity of distinguishing individual from ensemble measurements appear as important ingredients that have been overlooked in some of the theoretical literature.

In this letter we calculate the magnetic susceptibility of noninteracting electrons at finite temperatures in clean regular geometries (i.e. squares and circles) for individual systems as well as for ensembles. We use semiclassical approximation and classical perturbation theory since the magnetic fields involved are not big enough to modify the classical trajectories significantly. We explore the validity of our assumptions and analytical results with numerical calculations. We compare the results obtained for ensembles of regular structures with those of chaotic billiards, finding important quantitative differences. We show that, within a semiclassical approach, finite temperature induces a cut off on the classical trajectories considered, and therefore clean systems can provide a good description of the ballistic regime. This is the case for the experimental conditions of Ref. \[6\] and therefore our model yields results in good agreement with the measurements.

We consider an ensemble of isolated two-dimensional systems at temperature $T$. For each member of the ensemble (with $N$ electrons and area $V$) the magnetic susceptibility $\chi$ is given by the change of the free energy $F(T, N, H)$ under the effect of a magnetic field, \[1\]

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

The necessity of using the canonical ensemble for isolated mesoscopic systems, and the physical differences with the grand-canonical ensemble (GCE, where the system responds to the magnetic field with a fixed chemical potential $\mu$), are some of the important concepts that recently emerged in the context of persistent currents \[8\]. On the other hand, calculations in the GCE are more easily performed due to the simple form of the thermodynamic potential \[2\]

$$\Omega(T, \mu, H) = -\frac{1}{\beta} \int dE \rho(E) \ln (1 + \exp [\beta (\mu - E)]) ,$$

in terms of the density of states $\rho(E) = -(2/\pi) \Im g(E)$. The factor of 2 takes into account spin degeneracy, $\beta = 1/k_B T$, and $g(E)$ is the trace of the Green function $G_E(r', r)$, i.e.

$$g(E) = \int dr G_E(r, r) .$$  

Separating $\rho$ into a mean (Weyl) part, which is field independent, and an oscillating part, $\rho(E) = \rho^0(E) + \rho^{osc}(E)$, we define a mean chemical potential $\mu^0$ from $N = \int dE \rho(E)f(E-\mu) = \int dE \rho^0(E)f(E-\mu^0)$. ($f$ is the Fermi-Dirac distribution function.) Considering that $\rho^{osc} \ll \rho^0$, it has been shown [4]

$$F(N) = F^0 + \Delta F^{(1)} + \Delta F^{(2)},$$

where $F^0 = \mu^0 N + \Omega^0(\mu^0)$ and $\Delta F^{(1)} = \Omega^{osc}(\mu^0)$. We define $\Omega^0$ and $\Omega^{osc}$ by respectively $\rho^0$ and $\rho^{osc}$ instead of $\rho$ in Eq. (2). The second-order term is [4]

$$\Delta F^{(2)} = \frac{1}{2\rho^0(\mu^0)} \left[ \int dE \rho^{osc}(E) f(E-\mu^0) \right]^2.$$  

$F^0$ is field independent and does not contribute to $\chi$. $\Delta F^{(1)}$ gives the susceptibility in a GCE with chemical potential $\mu^0$. In disordered systems it vanishes under impurity average, and we will show that it is also the case within the averages of our semiclassical model.

We will calculate $\rho^{osc}$ from the semiclassical expansion of the Green function. Except for a logarithmic singularity when $r' \rightarrow r$, which yields the smooth part $\rho^0$ of $\rho$, the semiclassical Green function has the generic form [10]

$$G^\text{sc}_E(r',r) = \sum_t D_t \exp \left[ \frac{i}{\hbar} \left( S_t - \left( \eta_t - \frac{1}{2} \pi \right) \right) \right],$$

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

Within our semiclassical approach, the free energy corrections are 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 $\beta$). It can be shown [11] that the $T=0$ contribution to $\Delta F^{(1)}$ of a trajectory is reduced by a temperature-dependent 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 of $R^2(T)$ is needed for $\Delta F^{(2)}$. For long trajectories and high temperatures, $R(T)$ results in an exponential suppression and therefore the fluctuating part of the free energy, and $\chi$, are dominated by trajectories with $L_t \leq L_c$, which will be the only ones considered in our analysis. (We will not write $R(T)$ and $R^2(T)$ in the equations that follow.)

The standard route to obtain $\rho^{osc}$ from $G^\text{sc}_E$ is to evaluate the integral of Eq. (3) by stationary-phase approximation. This selects the trajectories which are not only closed in configuration space ($r' = r$), but also closed in phase space ($p' = p$), i.e. periodic orbits. When these latter are [well] isolated the Gutzwiller Trace Formula [10] is obtained. For integrable systems, periodic orbits come in continuous families corresponding to the rational invariant tori (Berry-Tabor Trace Formula [12]). The difficulty in following this approach in our case stems from the fact that in calculating $\chi$ for small fields, one is actually looking at the effect of a small perturbation on rational tori. The Poincaré-Birkhoff theorem states that, as soon as the field is turned on, generically (the circular billiard being a notable exception) all rational tori (i.e. all families of periodic orbits) are instantaneously broken,
leaving only two (one stable, one unstable) isolated periodic orbits. On the one hand, the physical effect which generates $\chi$ is the breaking of the rational tori, so that just ignoring this, i.e. using the Berry-Tabor Formula, is certainly inadequate. On the other hand, for $H \to 0$, the remaining orbits are not sufficiently well isolated to apply the Gutzwiller Trace Formula. Therefore, a uniform treatment of the perturbing field is needed, where not only orbits that are closed in phase space are taken into account, but also trajectories closed in configuration space which can be traced to periodic orbits when $H \to 0$.

In squares (of side $a$), due to the simplicity of the geometry, such a uniform treatment is possible since we can perform the corresponding integrals exactly. For $H = 0$, $\eta_t$ is twice the number of reflections, and $D_t = \alpha/L_t^{1/2}$ with $\alpha = -\pi(2m)^{3/4}/[(2\pi \hbar)^{3/2}E^{1/4}]$. One way to obtain this result is to use the method of images and express $G_E$ in terms of the free Green function $G_E^0$ as

$$G_E(r', r) = G_E^0(r', r) + \sum_{r_i'} \epsilon_i G_E^0(r_i', r),$$

where the $r_i'$ are all the mirror images of $r'$ by any combination of symmetries across the sides of the square, and $\epsilon_i = \pm 1$ depending on the number of symmetries needed to map $r'$ on $r_i'$. The long-range asymptotic behavior of the two-dimensional free Green function $G_E^0(r', r) \simeq \alpha \exp \left[i(k|r'_i - r| - \pi/4)/|r'_i - r|^{1/2}\right]$ can be used for the images [13].

For sufficiently weak magnetic fields, one may keep in Eq. (8) the zero-order approximation for $D_t$, and use the first-order correction $\delta S$ to the action. For a closed orbit enclosing an algebraic area $A$, classical perturbation theory yields $\delta S = (e/c)H A$ for low fields and high energies, such that the cyclotron radius of the electrons is much larger than the typical size of the structure.

We now specify the contribution $\rho_{11}$ [to $\rho^{\text{osc}}$] 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 it (1,1) since the trajectories bounce once on each side of the square (upper inset, Fig. 1). Their length is $L_{11} = 2\sqrt{2}a$. This family gives the main contribution to the experiment of Ref. [6]. The contribution of other families is obtained essentially in the same way. However, strong flux cancellation occurring for other primitive orbits makes their contribution irrelevant in the case of the square, even for very low temperatures [11,14]. Using as space coordinates $x_0$, which labels the trajectory, $s$ the distance along the trajectory, and the index $\epsilon = \pm 1$ specifying the sense of motion [15], the area is simply $A_s(x_0) = \epsilon 2x_0(a - x_0)$. Inserting $A$ in Eq. (5) we have $\rho_{11}(H) = \rho_{11}(H=0)\mathcal{C}(H)$, where $\rho_{11}(H=0) = -8a^2\alpha \sin (kL_{11} + \pi/4)/L_{11}^{1/2}$ is the unperturbed contribution and

$$\mathcal{C}(H) = \int_0^a dx_0 \cos \left(\frac{2e}{\hbar c}Hx_0(a - x_0)\right) = \frac{1}{\sqrt{2}\varphi} \left[\cos(\pi \varphi)C(\sqrt{\pi \varphi}) + \sin(\pi \varphi)S(\sqrt{\pi \varphi})\right].$$

$C$ 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 $\Phi_0 = \hbar c/e$. For $\varphi \geq 1$ the Fresnel integrals can be replaced by their asymptotic value $1/2$, which amounts to evaluating $\mathcal{C}(\varphi)$ by stationary phase, i.e. $\mathcal{C}(\varphi) = \cos(\pi \varphi + \pi/4)/\sqrt{4\varphi}$. This expression however diverges for $H \to 0$, while $\mathcal{C}(0) = 1$.

The contribution of the (1,1) family to $\Delta F^{(1)}$ yields, in leading-order in $k_Fa$
\[
\chi^{(1)} = \frac{3}{(\sqrt{2}\pi)^{5/2}} (k_F a)^{3/2} \sin \left( k_F L_{11} + \frac{\pi}{4} \right) \frac{d^2\mathcal{C}}{d\varphi^2}.
\]

(9)

Therefore, the susceptibility of a given square can be paramagnetic or diamagnetic (Fig. 1) and its typical magnitude is much larger than \(\chi_L\), with \(-\chi_L = -e^2/(12\pi mc^2)\) being the two-dimensional Landau susceptibility. Clearly, \(\chi^{(1)}\) vanishes under average if the dispersion of \(k_F a\) across the ensemble is of the order of \(2\pi\). The average \(\chi\) is then given by the contribution of the \((1,1)\) family to \(\Delta F^{(2)}\)

\[
\langle \chi \rangle = -\frac{3}{(\sqrt{2}\pi)^3} k_F a \frac{d^2\mathcal{C}^2}{d\varphi^2}.
\]

(10)

The average susceptibility (solid line, Fig. 3) is paramagnetic at \(H = 0\) and for low fields it oscillates with an overall decay of \(1/\varphi\). The divergent susceptibility obtained from \(\mathcal{C}^S\) (dotted line) provides a good description of \(\chi\) for \(\varphi \geq 1\). For ensembles with a wide distribution of lengths \(a\) (in Ref. [6] the dispersion in size across the array is estimated between 10 and 30%) a second average in \(d^2\mathcal{C}^2/d\varphi^2\) should be performed. (Since the scale of variation of \(\mathcal{C}\) with \(a\) is much slower than that of \(\sin (k_F L_{11})\) we can effectively separate the two averages.) The low-field oscillations of \(\langle \chi \rangle\) are suppressed under the second average (done for a gaussian distribution with a 30% dispersion, dashed line), while the zero-field behavior remains unchanged.

We checked the semiclassical results calculating the first 1500 eigenenergies of a square in a magnetic field by direct diagonalization. At \(T = 0\) the free energy reduces to the total energy and \(\chi\) is dominated by big paramagnetic singularities at the level-crossings of states belonging to different symmetry classes and at small avoided-crossings between states with the same symmetry [3]. These peaks are compensated once the next state is considered, and therefore disappear at finite temperature where the occupation of nearly degenerate states becomes almost the same. Temperature regularizes the \(T = 0\) singular behavior, and of course, describes the physical situation. We include it by calculating the partition function \(Z = \exp [-\beta F]\) from a recursive algorithm [16,11]. The results for individual squares are in excellent agreement with Eq. (9), the oscillations as a function of \(k_F L_{11}\) (and \(\varphi\)) clearly shown in Fig. 1. The average values also agree with our analytical findings (Fig. 2).

Ref. [6] yielded a paramagnetic susceptibility at \(H = 0\) with a value of approximately 100 (within a factor of 4) in units of \(\chi_L\). For the two electron densities \(n_e = 10^{11}\) and \(3\times10^{11} cm^{-2}\) of the experiment, the factor \(4\sqrt{2}/(5\pi)k_F a\) from Eq. (10) gives respectively a susceptibility of 130 and 220, that when temperature is considered (through \(R^2(T = 40 mK)\)) become 60 and 170, in good agreement with the measurements. The field scale for the decrease of \(\langle \chi(H=0)\rangle\) is of the order of one flux quantum through each square, in reasonable agreement with our theoretical findings. The temperature scale for the decrease of the susceptibility was identified as given by the inverse time-of-flight \(v_F/a\), which is the same scale \(L_t/L_c\) that we find.

Squares constitute a generic example of an integrable system perturbed by a magnetic field. It is interesting to compare our results with two extreme cases: circles (which remain integrable under the perturbation) and completely chaotic systems. Expressing the Hamiltonian of a circle (of radius \(a\)) in action-angle variables [17], \(\rho^\text{osc}\) can be written as a sum.
over families of periodic trajectories [12]. Within our finite-temperature approach we restrict ourselves to the shortest ones, the whispering-gallery trajectories who turn only once around the circle in coming to the initial point after $M$ bounces. Their contribution to $\rho^{\text{osc}}$ is

$$
\rho_{\text{wg}}(H) = \sum_{M=3}^{\infty} \rho_M(H=0) \cos \left( \frac{eH}{\hbar c} A_M \right).
$$

(11)

$$
\rho_M(H=0) = \sqrt{8mL_M^3/2} \sin \left( \frac{kL_M + \pi}{2} - \frac{3\pi M}{2} \right) \sin \left( \frac{\pi}{M} \right) \sin^2 \left( \frac{2\pi}{M} \right)/M \approx 0.7.
$$

The sums over $M$ are rapidly convergent, indicating the dominance of the first few periodic orbits.

Squares and circles give the same dependence on $k_F a$ for $\chi^{(1)}$ and $\langle \chi \rangle$. This generic behavior for integrable systems can be traced to the $k^{-1/2}$ dependence of the contribution to $\rho^{\text{osc}}$ most sensitive to the magnetic field. The numerical prefactors depend on the specifics of the geometry. The main contribution to $\chi$ at $H=0$ comes from interference between pairs of time-reversed trajectories. In the circle all periodic orbits within a family have the same area, while for squares the dominant family $(1,1)$ also includes periodic orbits with small enclosed area. This difference results in a larger value of $\langle \chi(H=0) \rangle$ (by a factor of 10) for the circle and the absence of the $1/\varphi$ damping of the low field oscillations.

For chaotic systems (of typical length $a$) with hyperbolic periodic orbits the Gutzwiller Trace Formula provides the appropriate path to calculate $\rho^{\text{osc}}$. When only a few short periodic orbits are important, $\chi$ can have any sign and its magnitude is of the order of $k_F a \chi_L$ [19]. Extending this analysis to the case of an ensemble of chaotic systems we obtain $\langle \chi \rangle \propto \chi_L$. The individual $\chi$ are larger, by a factor $(k_F a)^{1/2}$ in regular geometries than in chaotic systems [20]. For $\langle \chi \rangle$ the difference is even larger (factor $k_F a$). This is due to the large oscillations of $\rho$ in regular systems induced by families of periodic trajectories. 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). This assures that small variations in the geometry of the clean systems that we have considered will not be relevant.

We believe that measuring the susceptibility in different geometries will be of high interest in order to understand the applicability of simple noninteracting semiclassical models to actual microstructures.

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FIGURES

FIG. 1. Magnetic susceptibility of a square as a function of $k_Fa$ from numerical calculations at zero field and a temperature equal to 10 level-spacings. The number of electrons is $N = (k_Fa)^2/(2\pi)$. The dashed line is the envelope of the oscillations (in $k_FL_{11}$) of our semiclassical approximation with the temperature correction factor $R(T)$. 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 $k_FL_{11}$) of $\chi$ as a function of the flux through the sample from Eq. (1) (dashed) and numerics (solid).

FIG. 2. Average magnetic susceptibility for an ensemble of squares from Eq. (10) (solid) and from the stationary-phase integration $C_S$ (dotted). Dashed: average over an ensemble with a large dispersion of sizes (see text), Thick dashed: average from numerics. Inset: average susceptibility as a function of $k_Fa$ for various temperatures (4, 6 and 10 level spacings) and a flux $\varphi = 0.15$, from Eq. (10) (dashed) and numerics (solid).