Orbital magnetism in ensembles of parabolic potentials

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We study the magnetic susceptibility of an ensemble of noninteracting electrons confined by parabolic potentials and subjected to a perpendicular magnetic field at finite temperatures. We show that the behavior of the average susceptibility is qualitatively different from that of billiards. When averaged over the Fermi energy the susceptibility exhibits a large paramagnetic response only at certain special field values, corresponding to commensurate classical frequencies, being negligible elsewhere. We derive approximate analytical formulas for the susceptibility and compare the results with numerical calculations. [S1063-651X(98)04110-5]

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The interest in the magnetic properties of ensembles of mesoscopic systems has increased considerably in the last years [1,2]. The main motivation for the theoretical investigations recently carried out is the experimental results obtained by Levy *et al.* [3] for an ensemble of square billiards in the ballistic regime. It is now understood that, when averaged over a large ensemble of similar systems, the magnetic susceptibility χ of regular systems is enhanced with respect to the Landau susceptibility χ_L due to the coherent contribution of families of periodic orbits. For chaotic systems χ is usually small, of the order of χ_L, but bifurcations might play an important role in increasing the susceptibility [4]. Also, for square billiards, the averaged susceptibility is always paramagnetic at low magnetic fields. This behavior seems to be generic of regular billiards [1].

The purpose of this Brief Report is to study the magnetic susceptibility of an ensemble of noninteracting two-dimensional electron gas confined by parabolic quantum wells at finite temperatures. The interest in such confined mesoscopic systems was renewed both by the recent experimental developments in condensed matter [5] and its importance in the theoretical study [6] of trapped ion experiments [7]. We show that the behavior of χ as a function of the magnetic field B and Fermi energy μ is very different from that of billiards when ensemble averages are considered. The main reason for the this strong difference resides on the resonances exhibited by the system as the magnetic field is varied. These resonances are peculiar of harmonic potentials and are due to the degeneracy of the tori on the energy shell. The magnetic response of a single harmonic oscillator at zero temperature in a magnetic field has been considered before by Prado *et al.* [4] and Németh [8]. In this work we derive simple analytic expressions for χ that are directly amenable of ensemble averages.

In the canonical ensemble the magnetic susceptibility per particle $\chi = -(1/N)\partial^2 F/\partial B^2$ measures the sensitivity of the Helmholtz free energy F to the magnetic field B. For a noninteracting model F can be computed exactly if the number of particles N and the temperature T are not too large [9]. However, for large N and temperatures of the order of the the mean level spacing (in units of Boltzmann constant k_B), χ can be computed quite accurately by using an auxiliary grand-canonical potential where the average number of particles is kept fixed by properly adjusting the chemical potential for each value of the magnetic field [10]. The grand-canonical potential is given by

$$V = -\frac{1}{\beta}\int dE\ \rho(E)\ln(1+e^{\beta(\mu-E)}), \tag{1}$$

where ρ is the density of states, $\beta = 1/k_B T$ and μ is the chemical potential. In the semiclassical limit ρ can be separated into a mean term ρ^0 plus oscillatory contributions $\rho^{\rm osc}$ that are usually written in terms of period orbits [11]. After substituting $\rho = \rho^0 + \rho^{\rm osc}$ in Eq. (1), the grand-canonical potential also separates into $V^0(\mu) + V^{\rm osc}(\mu)$. Following Ullmo *et al.* [1] we define a mean chemical potential μ^0 from $N = \int dE \rho(E) f(E-\mu) = \int dE \rho^0(E) f(E-\mu^0)$ where $f(x) = 1/(1+e^{\beta x})$ is the Fermi-Dirac distribution function. Using the thermodynamical relation $F(N) = V(\mu) + \mu N$ with $\mu = \mu(N)$ obtained from the equations above, it can be shown [10] that, in the semiclassical limit, the free energy can be written as a sum of three terms, $F = F^0 + \Delta F^1 + \Delta F^2$, where $F^0 = V^0(\mu^0) + \mu^0 N$ does not depend on the magnetic field B, $\Delta F^1 = V^{\rm osc}(\mu^0)$ and

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

In the case of a parabolic confinement, the Hamiltonian of an electron of charge e and effective mass m^* can be written directly in terms of action variables as [12] $H(\mathbf{I}) = \mathbf{\Omega}\cdot\mathbf{I}$ with $\Omega_1 = \frac{1}{2}(\xi_+ + \xi_-)$, $\Omega_2 = \frac{1}{2}(\xi_+ - \xi_-)$ and $\xi_\pm = \sqrt{(\omega_1 \pm \omega_2)^2 + e^2 B^2/m^{*2}}$. The quantum mechanical energy levels are therefore given by $E_{k_1 k_2} = \hbar\Omega_1(k_1 + 1/2) + \hbar\Omega_2(k_2 + 1/2)$. To compute the ρ^0 and ρ^{osc} we follow Berry and Tabor [13] and write the semiclassical density of states as

$$\rho(E) = 2\sum_{\mathbf{m}} \delta(E - H(\mathbf{I} = \mathbf{m} + 1/2)), \tag{3}$$

where $\mathbf{m} = (m_1, m_2)$ and the factor 2 takes care of spin degeneracy. Using the Poisson sum formula we find $\rho^0(E) = 2E/(\hbar^2\omega_1\omega_2)$ and

$$\rho^{\mathrm{osc}}=\frac{2}{\hbar^2}\sum_{\mathbf{m}}{}' \; e^{-i\pi(m_1+m_2)}\rho_{\mathbf{m}}, \tag{4}$$

with

$$\rho_{\mathbf{m}}=\int d\xi \frac{e^{2\pi i\mathbf{m}\cdot\mathbf{I}(\xi)/\hbar}}{|\boldsymbol{\omega}(\mathbf{I}(\xi))|}, \tag{5}$$

where ξ varies along the energy surface in the (I_1,I_2) plane of the action variables. The prime above the summation symbol means that the term $(m_1,m_2)=(0,0)$ (responsible for ρ^0) is excluded. Explicitly we get $I_1=E/\Omega_1-\xi\Omega_2/\Omega$ and $I_2=\Omega_1\xi/\Omega$ for $0\leqslant\xi\leqslant E\Omega/(\Omega_1\Omega_2)$ with $\Omega\equiv\sqrt{\Omega_1^2+\Omega_2^2}$. For generic Hamiltonians the integration over ξ can performed within the stationary phase approximation and gives a semiclassical expression for ρ^{osc}. In the present case the integration can be carried out exactly and results in

$$\rho^{\mathrm{osc}}=\sum_{\mathbf{m}}{}' \; \frac{2(-1)^{m_1+m_2}e^{(i\pi E/\hbar\Omega_1\Omega_2)(m_2\Omega_1+m_1\Omega_2)}}{\pi\hbar(m_2\Omega_1-m_1\Omega_2)} \times\sin\left[\frac{\pi E}{\hbar\omega_1\omega_2}(m_2\Omega_1-m_1\Omega_2)\right]. \tag{6}$$

Substituting the above expression for ρ^{osc} in the formulas for ΔF^1 and ΔF^2 we get

$$\Delta F^1=\sum_{\mathbf{m}}{}'' \; \frac{(-1)^{m_1+m_2}}{\hbar^2\omega_1\omega_2(\gamma_2-\gamma_1)}\frac{4\pi\mu^{02}}{\beta}\left[\frac{\sin(\gamma_2)(1-\delta_{m_20})}{\gamma_2\sinh(\pi\gamma_2/\mu^0\beta)} - \frac{\sin(\gamma_1)(1-\delta_{m_10})}{\gamma_1\sinh(\pi\gamma_1/\mu^0\beta)}\right] \tag{7}$$

and

$$\Delta F^2=\frac{1}{2\rho^0}\left\{\sum_{\mathbf{m}}{}'' \; \frac{(-1)^{m_1+m_2}}{\hbar^2\omega_1\omega_2(\gamma_2-\gamma_1)}\frac{4\pi\mu^0}{\beta} \times\left[\frac{\cos(\gamma_2)(1-\delta_{m_20})}{\sinh(\pi\gamma_2/\mu^0\beta)}-\frac{\cos(\gamma_1)(1-\delta_{m_10})}{\sinh(\pi\gamma_1/\mu^0\beta)}\right]\right\}^2. \tag{8}$$

The double prime in the summations means that only the integers (m_1,m_2) in the upper half plane, minus the negative m_1 axis, are included. We have also defined $\gamma_i=2\pi\mu^0 m_i/(\hbar\Omega_i)$.

Both expressions for ΔF^1 and ΔF^2 can be simplified if one notes that, as the magnetic field is varied, the ratio Ω_1/Ω_2 passes densely through rational numbers, where all the classical orbits of the system are periodic. To those field values there also corresponds a large degeneracy of the energy levels. We therefore restrict our attention initially to the neighborhood of these values of B only. Let $B=B_{nm}$ be such that $\Omega_1=n\Omega_0$ and $\Omega_2=m\Omega_0$, i.e., $\Omega_1/\Omega_2=n/m$ and $\Omega_0=\sqrt{\omega_1\omega_2/nm}$ is the frequency of the classical periodic orbits. At those points the denominator in Eqs. (7) and (8) vanishes for all (m_1,m_2) of the form (pn,pm) for all $p>0$ and we see that the main contributions to ΔF^1 and ΔF^2 come from these *resonant* terms. Defining the function

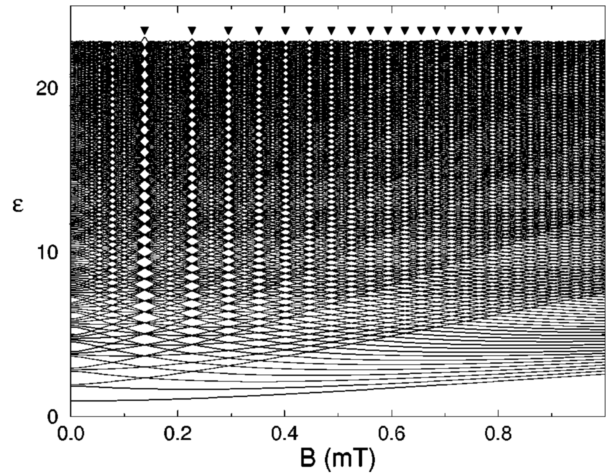

FIG. 1. The first 290 single particle energy levels normalized to $\epsilon=E/(\hbar\omega_1)$ as a function of the magnetic field B. The triangles on top indicate the resonances with $m=1$ and $n=2,\ldots,20$.

$$S(B)=\frac{\sin[C(B)]}{C(B)}, \tag{9}$$

where $C(B)=\frac{1}{2}(\gamma_2-\gamma_1)=(\pi\mu^0/\hbar\omega_1\omega_2)(n\Omega_2-m\Omega_1)$ vanishes at B_{nm}, we get, after rearranging the trigonometric functions and considering only the term $p=1$, the following approximated expressions:

$$\Delta F^1=\frac{(-1)^{n+m}\mu^0R(\beta)}{\pi^2nm}\cos\left(\frac{2\pi\mu^0}{\hbar\Omega_0}\right)S(B) \tag{10}$$

and

$$\Delta F^2=\frac{\mu^0R^2(\beta)}{\pi^2nm}\sin^2\left(\frac{2\pi\mu^0}{\hbar\Omega_0}\right)S^2(B), \tag{11}$$

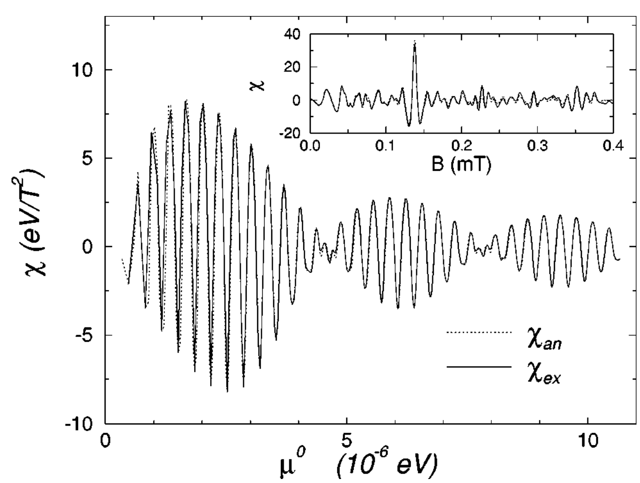

FIG. 2. Magnetic susceptibility χ as a function of μ^0 at $B=0$ and $T=0.3$ mK. The inset shows χ as a function of B for a single system, without any average, for the same temperature and $N=500$. In both cases the full line represents the numerical exact result and the dotted line shows the analytical calculation $(\chi^L+\chi^1+\chi^2)$.

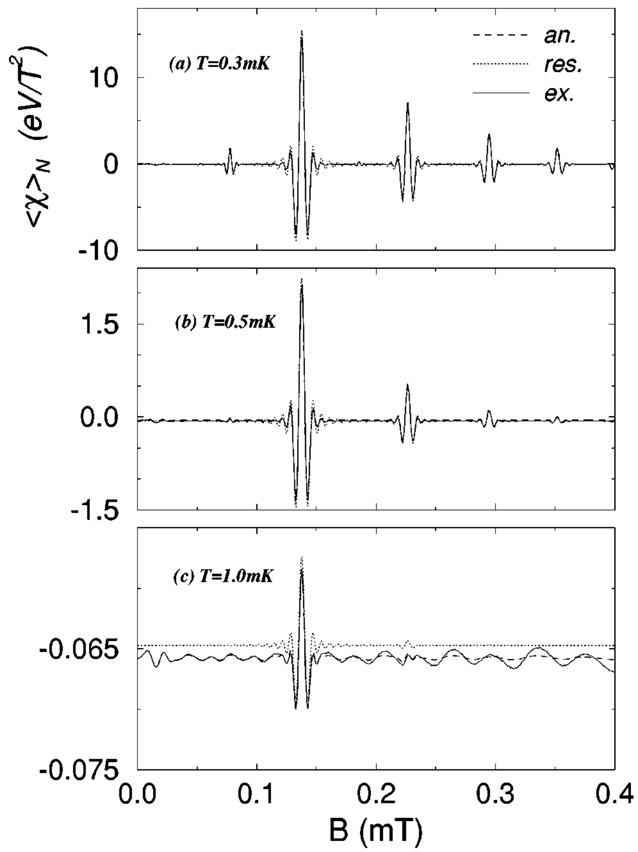

FIG. 3. Susceptibility averaged over N as a function of the magnetic field for three different temperatures. In all cases $N=500$, $\delta N/N=0.2$, the full line represents the exact result, the dotted line shows the resonant approximation, and the dashed line shows the full analytic formula, Eqs. (7) and (8).

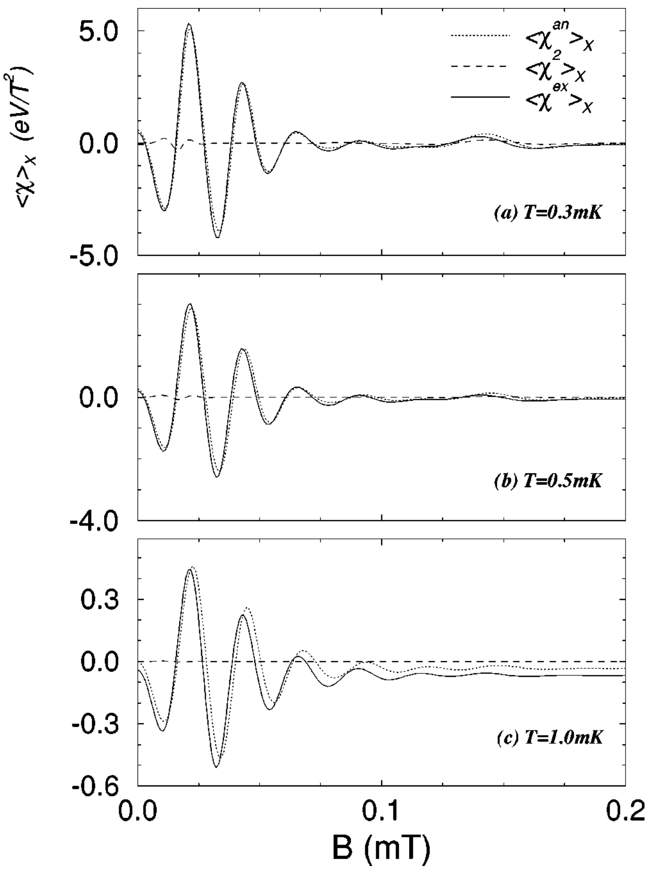

FIG. 4. *Size* averaged susceptibility (see text) as a function of the magnetic field for three different temperatures. In all cases $\delta x=0.1$, the full line represents the exact result and the dotted and dashed lines show the contributions of the full analytic calculation and that of χ^2 alone, respectively.

where $R(\beta)=(2\pi^2)/(\hbar\beta\Omega_0)\ \sinh^{-1}[(2\pi^2)/(\hbar\beta\Omega_0)]$ is a temperature dependent factor that diminishes exponentially the susceptibility for large T's *and* large Ω_0's. The dependence of the free energy on the magnetic field has been reduced to $S(B)$ and the magnetic susceptibility can be readily computed. We recall that the Landau susceptibility for the oscillator is given by [4] $\chi_L=-(e/m^*)^2\hbar^2/(6\mu^0)$.

The expressions just derived describe the behavior of a single system in the thermodynamic limit. In the experiment with square billiards of Levy *et al.* [3], however, only the average properties of an ensemble of systems were measured. The individual members of the ensemble, although very similar, present small differences among themselves. Besides, the number of particles confined in each of them might vary slightly. To account for these fluctuations further averages have to be performed [1]. As in the case of billiards [1] the oscillatory contribution of ΔF^1 to χ vanishes under an average over the Fermi energy, or number of particles, for dispersions $\delta\mu$ of the order of $\hbar\Omega_0$. The contribution of ΔF^2 remains for the parabolic potential as it does in the case of billiards. The main difference here is that, due to the fact that the density of states increases linearly with the energy, the contribution of ΔF^2 is of the same order in μ^0 than that of ΔF^1. Also, in terms of particle number, the relative dispersion $\delta N/N$ necessary to kill ΔF^1 falls as $1/\sqrt{N}$. Therefore, for large N's, even very small dispersions will effectively wash out ΔF^1. The resulting susceptibility, after performing the average, is

$$\langle\chi\rangle_N=-\frac{\mu^0}{2\pi^2 Nnm}R^2(\beta)\frac{\partial^2 S^2(B)}{\partial B^2}. \qquad (12)$$

Therefore, since $\partial^2 S^2(B)/\partial B^2$ is proportional to N and has a negative peak at B_{nm}, χ exhibits a positive peak at each resonance whose strength goes as μ^0/nm.

In what follows we present numerical calculations performed with $\omega_1=5.4\times10^8\ \mathrm{s}^{-1}$, $\omega_2=0.9\omega_1$, and $m^*=0.067m_e$, which is the electron effective mass for a GaAs quantum well. Figure 1 shows the first 290 energy levels as a function of the magnetic field B. The arrows on top indicate the position of the most relevant resonances. Figure 2 shows χ as a function of μ^0 at $B=0$ for a single system, without the average. The inset shows χ as a function of B for 500 particles, corresponding to approximately $\mu^0=7.5\times10^{-6}$ eV. In both cases $T=0.3$ mK, the full line represents the numerical exact result and the dotted line shows the result derived from Eqs. (7) and (8). The agreement between exact and analytic results is very good. The approximate formulas, Eqs. (10) and (11) also give very accurate results for χ close to the resonances. Figure 3 shows $\langle\chi\rangle_N$, the susceptibility averaged over particle number, as a function of B for $N=500$ and dispersion $\delta N/N=0.2$ computed directly from the energy levels (full line), from the resonant formula (12) (dotted line), and from the full analytic expression Eqs. (7) and (8) (dashed line) for three different values of the temperature. The last two curves also include the contribution of χ_L. Once again we found an excellent agreement between the exact and approximate calculations (notice that the exact and analytical curves involve the separate calculation of χ for various N's before the average is performed).

We finally consider averages over different confining potentials. In order to keep the potentials integrable and not to introduce too many parameters we consider each member of the ensemble to have $\omega_1 = x\omega_{10}$ and $\omega_2 = x\omega_{20}$, with a Gaussian distribution of x around $\bar{x}=1$. This can be viewed as a *size* average, since x changes the available area in coordinate space without changing the shape of the potential. In what follows we use an extra index 0 to indicate quantities computed with $x=1$. Keeping the number N of particles fixed we see that $\mu^0 = \hbar\sqrt{Nx^2\omega_{10}\omega_{20}} = x\mu_0^0$ and $\Omega_0(B) = x\Omega_{00}$. Therefore, the oscillations in Eqs. (10) and (11), which depend on the ratio μ^0/Ω_0, are not affected by the averaging. However, since $\Omega_i(B) = x\Omega_{i0}(B/x)$, $S(B) = S_0(B/x)$ and averaging over x is equivalent to averaging over B/x. Writing $x = 1 + \delta x$, $B/x \sim B - B\,\delta x$ we see that the average is not effective for small values of the magnetic field. Therefore, the resonant peaks at large B's tend to be smoothed out, enhancing the susceptibility at the nonresonant region, close to $B=0$ for the current value of the parameters. These regions are described approximately by Eq. (7) with $(m_1, m_2) = (1,1)$ and show an oscillatory behavior with frequencies γ_1 and γ_2. Expanding $\gamma_i(B/x) \sim \gamma_i(B) - B\,\delta x\,\gamma_i'$ and imposing $|\gamma_i(B/x) - \gamma_i(B)| = 2\pi$ we find that the oscillations in χ die out for $eB/m^* \sim \sqrt{\hbar\bar{\Omega}(\omega_1^2 - \omega_2^2)/(\mu_0^0|\delta x|)}$ where $\bar{\Omega}$ is the smallest between Ω_1 and Ω_2. This is confirmed by the numerical data displayed in Fig. 4 for $\delta x = 0.1$ and different temperatures. Since the resonances are washed out by the average, we believe that the introduction of small anharmonicities in the potentials would not affect the results.

In conclusion, the magnetic response of an ensemble of two-dimensional electron gases confined by parabolic potentials is qualitatively different from that of an ensemble of billiards. The main features of the problem can be understood with the help of a *resonant* approximation for the density of states. For an ensemble of identical quantum wells, each holding slightly different number of electrons, the magnetic response is enhanced only at the resonances. When a dispersion in the size of the oscillators is included, the sharp response at the resonances are smoothed out but the susceptibility at low fields remains oscillatory as a function of the Fermi energy, and not necessarily paramagnetic as in the case of billiards. We emphasize that the nature of our approximations are different from those of Ref. [1], since here it is validy for all values of B, not only in the limit of small fields. The large peaks exhibited by the susceptibility at the resonances are very peculiar of the oscillator. The average density of states ρ^0, on the other hand, generally depend on the energy for smooth potentials, playing an important role in balancing the relative contributions of ΔF^1 and ΔF^2 at low temperatures. We notice that the oscillator parameters and magnetic field can be scaled in order to allow for experimentally accessible values. If the frequencies are both multiplied by α, the Fermi energy, the susceptibility, and the magnetic field are also multiplied by α, whereas the density of states scales as $1/\alpha$. For $\alpha = 10^3$, for instance, we would still be considering fields of the order of 0.1 T.

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