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Effects of finite temperature in ballistic quantum dots

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Abstract

We studied the effects of finite temperature in the magnetic susceptibility of a system of N non-interacting electrons in a homogeneous magnetic field and in a smooth confinement potential: the two-dimensional harmonic oscillator. Different exact ensemble calculations are considered and discussed: canonical (N fixed), canonical via grand-canonical (N average fixed) and partial canonical ensembles. We compute a Gaussian average of the susceptibility over the number of particles and another one over the size of system in order to compare our results with data of mesoscopic systems experiments. We conclude that it is fundamental to consider interactions between the particles in the theoretical analysis to obtain the temperature dependence of the experimental results. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

A lot of effort has been dovoted in the last few decades with the aim of knowing and characterizing properties of quantum mechanical systems that have their classical analogue as regular or chaotic systems. This is the main purpose of the field called Quantum Chaos [1]. Although the semiclassical theory has shown that classical dynamics has an important influence on quantum properties, this study is still far to be concluded.

The susceptibility of a system of charged particles was proposed as one property whose quantum behaviour should depend sensitively on the regularity of its classical analogue [2]. At the same time, the enormous progress in semiconductor technology has led to construct micro and nanometer devices, allowing mesoscopic experiments that have put still more interest in this subject.

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Recently Levy et al. [3] measured the orbital magnetic susceptibility of an ensemble of 10^5 isolated electron gas squares subjected to low magnetic field at subkelvin temperatures. These square structures resemble small electron billiards. The squares have 4.5 μm and are arranged in a regular array. The two studied samples have dispersion in size across the array about 30% for the first one and 10% for the second one. The average level spacing is between 3 and 5 mK.

In spite of the many theoretical efforts [4], one aspect remains without explanation: the behaviour of the measured susceptibility χ as a function of the temperature.

The purpose of this contribution is to study the finite temperature effects on χ for a very large range of magnetic field values for a non-interacting electron system in a smooth potential: the two dimensional harmonic oscillator. As known, this quadratic model is not only chaotic but even superregular. Different exact ensemble calculations are considered and discussed: canonical (N fixed), canonical via grand-canonical (N average fixed) and partial canonical ensembles. We computed a Gaussian average of the susceptibility over the number of particles and another one over the size of the system in order to simulate experimental situations. Results will be discussed in the last section.

2. The model

The single particle model consists of one electron (effective mass m and electric charge $-e$) confined in a two dimensional harmonic potential and subjected to a constant magnetic field perpendicular to the movement plane. The Hamiltonian form is (SI system)

$$H = \frac{1}{2m}(\boldsymbol{p} + e\boldsymbol{A})^2 + \frac{1}{2}m\varphi_1^2 x^2 + \frac{1}{2}m\varphi_2^2 y^2. \tag{1}$$

The oscillator energy eigenvalue problem, first studied by Darwin [5], was solved by Schuh [6]:

$$E(n_1, n_2) = \hbar\left[\omega_+\left(n_1 + \tfrac{1}{2}\right) + \omega_-\left(n_2 + \tfrac{1}{2}\right)\right], \tag{2}$$

where $\omega_c = (e/m)B$ is the cyclotron frequency and

$$\omega_\pm = \frac{1}{2}\left(\sqrt{\omega_c^2 + (\varphi_1 + \varphi_2)^2} \pm \sqrt{\omega_c^2 + (\varphi_1 - \varphi_2)^2}\right). \tag{3}$$

The diamagnetic properties of this system were extensively studied by Nemeth at zero temperature [7].

The mean level spacing of the oscillator is $\Delta = (\hbar^2\varphi_1\varphi_2)/E$. It is not constant as in the case of billiards, but depends on the energy and therefore on the number of particles of the system. In our calculations, $\Delta/k_B = 3.7\,\mathrm{mK}/\varepsilon$ where $\varepsilon = E/\hbar\varphi_1$.

3. Finite temperature calculations

We consider an ensemble of isolated systems with N particles and constant temperature T. The definition of magnetization per particle as a function of the magnetic field is $m(B)=-(1/N)(\partial F/\partial B)_{N,T}$, where $F=-(1/\beta)\ln Z$ is the Helmholtz free energy, Z is the canonical partition function and $\beta=1/k_BT$. The magnetic susceptibility is simple $\chi(B)=(\partial m/\partial B)_{N,T}$.

As it is known, for zero temperature the only contribution to the susceptibility occurs at the level crossing between the Fermi level and the level above it. All the other level crossing contributions vanish one another. When the temperature grows up, all the levels can contribute to the susceptibility.

Because of the practical difficulty to perform the finite temperature canonical calculations, an alternative procedure is commonly adopted: to obtain $F(N,T)$ through the Legendre transformation of the grand canonical potential $\Omega(\mu,T)$, namely, $F=\Omega+\mu T$. Here μ, the chemical potential, is obtained such that $N=2\sum_{k=1}^{\infty} f(\varepsilon_k)$, where the Fermi function is $f(\varepsilon_k)=1/1+e^{\beta(\varepsilon_k-\mu)}$. It is worthwhile to remember that this is not an exact relation, but its validity depends on the relation between temperature and the level spacing of the system. So we get

$$m(B)= -\frac{1}{N}\frac{\partial}{\partial B}(\Omega+\mu N)_{\mathrm{fixed}\,N} = -\frac{2}{N}\sum_n \left[f(\varepsilon_n)\left(\frac{\partial \varepsilon_n}{\partial B}\right)\right]_{\mathrm{fixed}\,N} . \tag{4}$$

In fact, we do not keep fixed N, but we keep fixed $\langle N\rangle$, whose dispersion increases with temperature.

Thus, we consider three distinct possibilities of calculations: (a) complete exact canonical, (b) canonical through grand canonical and (c) partial exact canonical. In this last case we verify the effect of neglect system configurations where the number of particles with $-\frac{1}{2}$ spin is different from the number of particles with $+\frac{1}{2}$ spin. In order to implement item (a) we adopted the procedure of Brack et al. [8]. It consists of a recurrence relation that reduces tremendously the time computation, such that it becomes possible for larger N calculations. Typically, here we worked with systems of 20 or 50 particles and the magnetic field values from zero to fields where Landau levels were observed at least for the occupied energy levels.

In order to simulate experimental situations we evaluated the Gaussian average over the number of particles and independently averaged over the size of the system potential (see Fig. 1). The average on number of particles is given by ($P=N/2$):

$$\langle\chi\rangle(B,\bar{P})=\frac{1}{2\Delta\sqrt{\pi}}\sum_{P=0}^{\infty}\chi(B,P)\exp[-(P-\bar{P})^2/4\Delta^2]\,, \tag{5}$$

while the potential size average is defined by

$$\langle\chi\rangle(B,N)=\frac{1}{\sqrt{2\pi}\sigma}\int \exp[-(k-1)^2/2\sigma^2]\chi(B,N,k\varphi_1,k\varphi_2)\,\mathrm{d}k\,. \tag{6}$$

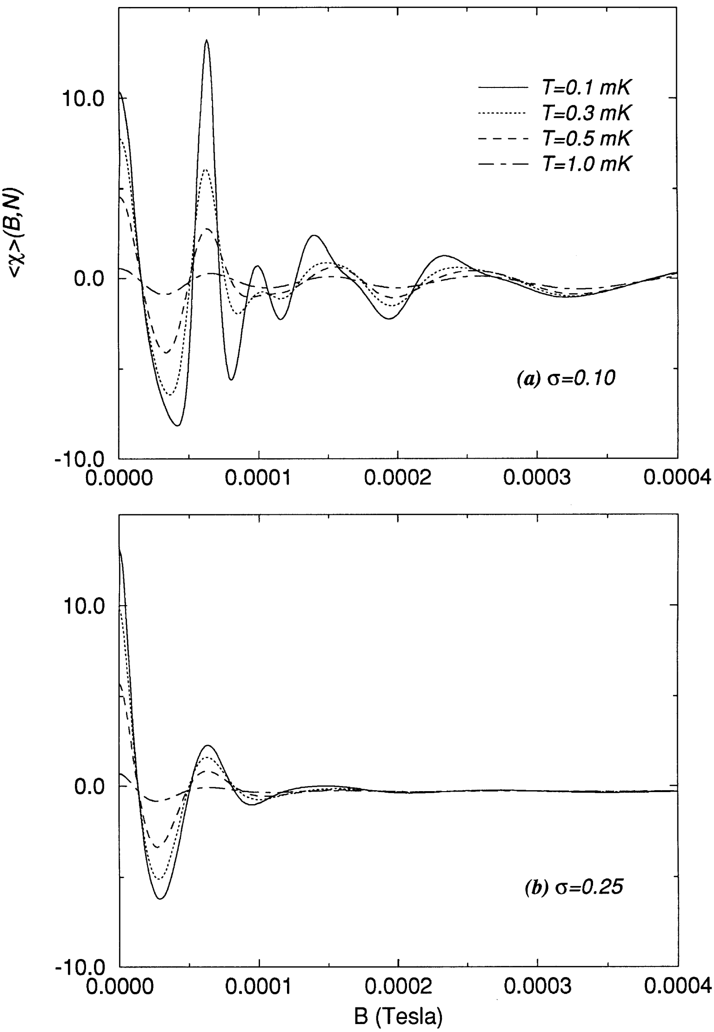

Fig. 1. Potential size Gaussian average as a function of the magnetic field (Eq. (6)) for a system of 24 particles, four temperature values, and (a) $\sigma = 0.10$ and (b) $\sigma = 0.25$.

There are other possible considerations that can be implemented, as for example, to keep constant the particle density instead of the number of particles in the last average, that can take us closer to experimental situations.

4. Results, discussion and conclusions

The first temperature effect that we observed was the spread of the narrow peaks observed at zero temperature (rigorously speaking, delta functions). With the temperature increase, the peak heights decrease as their widths grow until the curves $\chi \times B$

become completely smooth. For the oscillator potential, we see that the last peaks that survive are those at higher magnetic field, nearer and below the field values where the Landau levels are seen.

A good agreement was found among the three ensemble calculations studied. The approximation contained in the canonical through grand canonical ensemble does not manifest, because here, temperature effect on susceptibility is very fast, i.e., $\chi(B)$ is suppressed at a high rate, bigger than the experimentally observed one. The average over system number of particles speeds up, still more, this suppression. Now the average over the size of the potential system shows a distinct result. For $N=24$, we can see a paramagnetic peak for low field values followed by a diamagnetic valley for higher fields and then, one oscillating curve around the Landau susceptibility. This curve shape agrees with the experimental results at least where they are available (low field values). Meanwhile, when N is changed, this sequence of peaks may be inverted (diamagnetic–paramagnetic).

However, we could not reproduce the susceptibility behaviour with temperature measured by Levy et al. It leads us to conclude that an other physical ingredient(s) is (are) missing in our model and very probably the interaction between electrons is one of them.

Other possible considerations have been investigated as for example averages at constant particle density as well as the implementation of the two cited averages consecutively. Besides, one complete study as a function of different confinement potentials (square, circular and ellipse billiards) has been concluded and will be the subject of another work [9].

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