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Diamagnetism of Wigner oscillators

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Abstract. The orbital magnetic moment and the orbital magnetic susceptibility at finite temperature for a charged oscillator in a magnetic field of arbitrary strength are calculated exactly. Landau diamagnetism, a purely quantum mechanical non-vanishing diamagnetic susceptibility in the absence of a magnetic field and the Langevin formula are obtained as special cases.

1. Introduction

A particularly interesting thermodynamical property of solids is the contribution of conduction electrons to the magnetic susceptibility of a material. It is a remarkable fact that the contribution we expect on the basis of classical theory is identically zero. This may be shown by considering the classical Hamiltonian for a charged particle in a magnetic field:

$$H_c(\boldsymbol{r}, \boldsymbol{p}) = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right)^2 + V(\boldsymbol{r}) \tag{1}$$

and calculating the total energy

$$E = \int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{p}\,\rho[H_c(\boldsymbol{r}, \boldsymbol{p})]H_c(\boldsymbol{r}, \boldsymbol{p}) \tag{2}$$

where ρ is a distribution function depending only upon the energy of the particle. By performing the integration over momentum first and changing variables to $\boldsymbol{p}' = \boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r})/c$ we obtain a form which is entirely independent of the magnetic field. Therefore, the susceptibility must vanish given that it is directly proportional to the second derivative of the total energy with respect to the magnetic field. This result reflects the fact that classically a magnetic field does not change the energy of a charged particle but simply deflects it. This holds for any $V(\boldsymbol{r})$.

At a quantum mechanical level, however, the orbital motion of a charged particle in a magnetic field is quantised. The energy eigenvalues as well as the total energy depend upon the magnetic field and hence there is a corresponding contribution to the susceptibility: this is Landau diamagnetism [1, 2].

More general and realistic models must, however, include a potential in addition to the magnetic field, although in most cases this will considerably complicate the solution of the corresponding quantum mechanical problem. One such model which can be exactly solved is a localised Wigner oscillator [3, 4] in a magnetic field of arbitrary strength [5].

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We would like to show in this paper that it is possible to calculate exactly the magnetic moment of this system at finite temperature, reproducing other previously known results as special cases.

2. The partition function

The Hamiltonian for a localised Wigner oscillator in a magnetic field of arbitrary strength is

$$H=\frac{1}{2m}\left(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}\right)^2+\tfrac{1}{2}\lambda \boldsymbol{r}^2 \tag{3}$$

where the magnetic field is applied along the z axis and the gauge is chosen such that the vector potential $\boldsymbol{A}$ is given by $\frac{1}{2}\boldsymbol{B}\times\boldsymbol{r}$. The motion along the z axis is of no interest and thus will be omitted.

The corresponding Bloch density matrix in polar coordinates (r, θ) is [5]

$$C(\boldsymbol{r}\boldsymbol{r}_0\beta)=\frac{m\Omega}{2\pi\hbar\sinh(\beta\hbar\Omega)}\exp\left(\frac{-m\Omega}{2\hbar\sinh(\beta\hbar\Omega)}\{(r^2+r_0^2)\cosh(\beta\hbar\Omega) -2rr_0[\cos(\theta-\theta_0)\cosh(\beta\hbar\omega)+\mathrm{i}\sin(\theta-\theta_0)\sinh(\beta\hbar\omega)]\}\right) \tag{4}$$

where $\beta=1/kT$, ω is the Larmor frequency $eB/2mc$ and $\Omega^2=\omega^2+\lambda/m$.

The partition function is given by

$$Z(\beta)=\int_0^\infty\int_0^{2\pi} r\,\mathrm{d}r\,\mathrm{d}\theta\, C(\boldsymbol{r}\boldsymbol{r}\beta) \tag{5}$$

which by using (4) yields

$$Z(\beta)=\frac{1}{2[\cosh(\beta\hbar\Omega)-\cosh(\beta\hbar\omega)]}. \tag{6}$$

The eigenenergies can be easily obtained by rewriting (6) as $1/\{4\sinh[\beta\hbar(\Omega+\omega)/2]\sinh[\beta\hbar(\Omega-\omega)/2]\}$ and expanding in powers of exponentials:

$$Z(\beta)=\left(\sum_{l=0}^{\infty}\exp[-(l+\tfrac{1}{2})\beta\hbar(\Omega+\omega)]\right)\left(\sum_{n=0}^{\infty}\exp[-(n+\tfrac{1}{2})\beta\hbar(\Omega-\omega)]\right) \tag{7}$$

from which we can read the energy eigenvalues as $\varepsilon(l, n)=\hbar\Omega+(l+n)\hbar\Omega+(l-n)\hbar\omega$.

3. The orbital magnetic moment and the susceptibility

The thermally averaged orbital magnetic moment is $\langle\mu\rangle_0=-\partial F/\partial B$ where F is the free energy $-[\ln Z(\beta)]/\beta$ and therefore

$$\langle\mu\rangle_0=\frac{1}{\beta Z}\left(\frac{\partial\omega}{\partial B}\right)\left(\frac{\partial Z}{\partial\omega}\right)=\frac{\mu_{\mathrm{B}}}{\hbar\beta}\left(\frac{1}{Z}\frac{\partial Z}{\partial\omega}\right) \tag{8}$$

where μ_{B} is the Bohr magneton $e\hbar/2mc$. Using (6) we obtain

$$\langle\mu\rangle_0=-\tfrac{1}{2}\mu_{\mathrm{B}}\left(\{\coth[\beta\hbar(\Omega+\omega)/2]-\coth[\beta\hbar(\Omega-\omega)/2]\} +\frac{\omega}{\Omega}\{\coth[\beta\hbar(\Omega+\omega)/2]+\coth[\beta\hbar(\Omega-\omega)/2]\}\right) \tag{9}$$

which can also be written as

$$\langle\mu\rangle_0 = -\mu_B[(\omega/\Omega)\sinh(\beta\hbar\Omega) - \sinh(\beta\hbar\omega)]/\{2\sinh[\beta\hbar(\Omega+\omega)/2] \times \sinh[\beta\hbar(\Omega-\omega)/2]\}. \tag{10}$$

The orbital magnetic susceptibility $\chi_0 = \partial\langle\mu\rangle_0/\partial B$ equals $(\mu_B/\hbar)\partial\langle\mu\rangle_0/\partial\omega$. By using (9) we obtain

$$\chi_0 = \frac{1}{4\Omega^2}\beta\mu_B^2\Big(\operatorname{cosech}^2[\beta\hbar(\Omega+\omega)/2](\Omega+\omega)^2 + \operatorname{cosech}^2[\beta\hbar(\Omega-\omega)/2](\Omega-\omega)^2 - \frac{2}{\beta\hbar\Omega}\{\coth[\beta\hbar(\Omega+\omega)/2] + \coth[\beta\hbar(\Omega-\omega)/2]\}(\Omega^2-\omega^2)\Big). \tag{11}$$

These are exact results.

4. Special cases

We now consider some special cases of equations (9)-(11).

4.1. *Wigner oscillator*

(a) Low-temperature limits

$$\lim_{\beta\to\infty}\langle\mu\rangle_0 = -\mu_B\frac{\omega}{\Omega} \tag{12}$$

$$\lim_{\beta\to\infty}\chi_0 = -\frac{1}{\hbar\Omega}\mu_B^2\left(\frac{\Omega^2-\omega^2}{\Omega^2}\right). \tag{13}$$

From (12) we see that the effect of the harmonic oscillator potential is to lower the magnitude of the magnetic moment with respect to the potential-free case. From (13) we get $\chi_0 < 0$ and thus the Wigner oscillator is diamagnetic at low temperatures.

(b) High-temperature limits

$$\lim_{\beta\to 0}\langle\mu\rangle_0 = -\mu_B\frac{\hbar\omega\beta}{3} = -\mu_B^2\frac{B}{3kT} \tag{14}$$

$$\lim_{\beta\to 0}\chi_0 = -\mu_B^2\frac{1}{3kT}. \tag{15}$$

At high temperatures, we find both results to be independent of the harmonic oscillator potential and the susceptibility is furthermore independent of the strength of the magnetic field. The Wigner oscillator is also diamagnetic at high temperatures.

4.2. *Zero magnetic field*

$$\lim_{\omega\to 0}\langle\mu\rangle_0 = 0 \tag{16}$$

$$\lim_{\omega\to 0}\chi_0 = \tfrac{1}{2}\beta\mu_B^2\left[\operatorname{cosech}^2\left(\frac{\beta\hbar\Omega_0}{2}\right) - \frac{2}{\beta\hbar\Omega_0}\coth\left(\frac{\beta\hbar\Omega_0}{2}\right)\right] \tag{17}$$

where $\Omega_0^2 = \lambda/m$ is the harmonic oscillator frequency.

Equation (16) yields the expected result. Notice however from (17) that there is a non-vanishing diamagnetic susceptibility even in the absence of a magnetic field. This is a purely quantum mechanical effect [6] which persists even if we switch off the harmonic oscillator potential (i.e. a free charged particle):

$$\lim_{\substack{\omega\to 0\\ \Omega\to 0}} \chi_0 = -\mu_B^2 \frac{1}{3kT}. \tag{18}$$

It is important to observe that (18) is valid at all temperatures, whereas (15) is a high-temperature limit only.

(a) Low-temperature limits

$$\lim_{\substack{\omega\to 0\\ \beta\to\infty}} \langle\mu\rangle_0 = 0 \tag{19}$$

$$\lim_{\substack{\omega\to 0\\ \beta\to\infty}} \chi_0 = -\mu_B^2 \frac{1}{\hbar\Omega_0}. \tag{20}$$

Notice that (19) and (20) can also be obtained directly from (12) and (13).

(b) High-temperature limits

$$\lim_{\substack{\omega\to 0\\ \beta\to\infty}} \langle\mu\rangle_0 = 0 \tag{21}$$

$$\lim_{\substack{\omega\to 0\\ \beta\to\infty}} \chi_0 = -\mu_B^2 \frac{1}{3kT}. \tag{22}$$

4.3. *Charged particle in a magnetic field*

$$\lim_{\Omega\to\omega} \langle\mu\rangle_0 = -\mu_B\left(\coth(\hbar\omega\beta) - \frac{1}{\hbar\omega\beta}\right) = -\mu_B\left[\coth\left(\frac{\mu_B B}{kT}\right) - \frac{kT}{\mu_B B}\right] \tag{23}$$

$$\lim_{\Omega\to\omega} \chi_0 = -\mu_B^2\beta\left(-\operatorname{cosech}^2(\hbar\omega\beta) + \frac{1}{(\hbar\omega\beta)^2}\right). \tag{24}$$

Equation (23) is the Langevin formula.

(a) Low-temperature/strong field limits

$$\lim_{\beta\to\infty} \langle\mu\rangle_0 = \lim_{\omega\to\infty} \langle\mu\rangle_0 = -\mu_B \tag{25}$$

$$\lim_{\beta\to\infty} \chi_0 = \lim_{\omega\to\infty} \chi_0 = 0. \tag{26}$$

These results are valid for all field strengths at low temperatures or for all temperatures in strong fields.

(b) High-temperature/weak field limits

$$\lim_{\beta\to 0} \langle\mu\rangle_0 = \lim_{\omega\to 0} \langle\mu\rangle_0 = -\mu_B^2 \frac{B}{3kT} \tag{27}$$

$$\lim_{\beta\to 0} \chi_0 = \lim_{\omega\to 0} \chi_0 = -\mu_B^2 \frac{1}{3kT}. \tag{28}$$

This is Landau diamagnetism [1, 2] and is valid for all field strengths at high temperature or for all temperatures in weak fields.

5. Pauli paramagnetism

Although our main interest in this paper has been to study the diamagnetism of the Wigner oscillator, its special cases and limits, we can easily extend our treatment to include the paramagnetic effect of the spin of a charged particle. Let us consider electrons in particular.

To our main results (10) and (11) we must add

$$\langle\mu\rangle_s = \mu_B \tanh\left(\mu_B \frac{B}{kT}\right) \tag{29}$$

$$\chi_s = \mu_B^2 \operatorname{sech}^2\left(\mu_B \frac{B}{kT}\right)(kT)^{-1} \tag{30}$$

respectively. At high temperatures, the spin magnetic susceptibility is μ_B^2/kT, which is three times larger in magnitude than the orbital magnetic susceptibility and of opposite sign. An electron gas will therefore have a total susceptibility of $2\mu_B^2/3kT$ at high temperatures and will be paramagnetic. Most simple metals are in fact paramagnetic.

6. Conclusions

The principal results of this paper are equations (10) and (11). Besides being exact results, they correspond to the solution of a more general non-trivial quantum mechanical problem of electron crystallisation which naturally arises when a sufficiently strong Coulomb repulsion leads electrons to oscillate about lattice sites in harmonic potentials.

Even though genuine Wigner crystals have not yet been unambiguously identified, extensive work on highly compensated semiconductors in strong magnetic fields indicates the relevance of Wigner cystallisation. The results presented herein might find appropriate use in this important area of research in the near future.

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