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Pauli Paramagnetism Revisited

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Abstract The magnetization of an equilibrium system of non-interacting fermions with magnetic moments is re-examined, and for very large field strengths is expressed in a manner which is completely satisfactory both physically and mathematically.

1. INTRODUCTION

Since 1927 the phenomenon of Pauli paramagnetism[1] has been one of the pillars upon which the theory of metals rests, as well as a major accomplishment of quantum statistical mechanics. A simple model consists of a system of spin-1/2, charge-neutral fermions with mass m in thermal equilibrium and, if the spin and magnetic moment are taken in the same direction, the latter is just the Bohr magneton μ_0. For a uniform magnetic field H in the z-direction one finds the standard and well-known result for the magnetization[2,3]

$$M = \mu_0 (n_+ - n_-) \tag{1}$$

where in the limit of zero temperature the number densities of particles with spin up and spin down, respectively, are

$$n_\pm \simeq (4\beta^{3/2}/3\pi^{1/2}\lambda_T^3)(\mu \pm \mu_0 H)^{3/2} \tag{2}$$

Here we have denoted the chemical potential by μ, $\beta = (kT)^{-1}$, k is Boltzmann's constant, T is the absolute temperature, and the thermal wavelength is $\lambda_T = (2\pi\hbar^2\beta/m)^{1/2}$.

When $\beta\mu_0 H << 1$ the chemical potential is given by the Fermi

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energy, E_F, as $T \to 0$, within terms of order $\mu_0^2 H^2$. Expansion in Eqs. (1) and *(2)* then yields the results of Pauli paramagnetism

$$M \simeq \frac{3}{2} \frac{\mu_0^2 H}{E_F} n \ , \quad \chi_p = \frac{\partial M}{\partial H} \simeq \frac{3}{2} \frac{n\mu_0^2}{E_F} \ , N = N_+ + N_- \tag{3}$$

But what happens when the external field is very large, we can nolonger presume that $\beta\mu_0 H << 1$, and no longer make an expansion?

As H is increased considerably, and $\mu_0 H \to \mu$, one sees that $n_- \to 0^+$. This confirms our physical expectation that, for sufficiently large H, there will be essentially no particles in the spin-down state and the system saturates with almost all spins up. Unfortunately that is not the complete mathematical description provided by Eqs. (1) and (2), because as H continues to increase n_- becomes imaginary and these expressions are no longer physical. Although one can argue that n_- is to be discarded once it reaches 0^+, this hardly constitutes a satisfactory mathematical procedure. The fact that the chemical potential is a function of the field does not resolve the difficulty, either. As we shall see below, this means that the theory described by Eqs. (1) and *(2)* is only valid for field energies up to about 80% of $E_F(H=0)$, as is Implicit in the standard discussions[2].

It is true, of course, that it is quite difficult to encounter uniform magnetic fields large enough to give rise to this problem. But the points are those of mathematical principle and the soundness of the underlying theory of magnetism. Indeed, an examination of the corresponding relativistic theory, which motivated the present study and wlll be discussed elsewhere[13], indicates that field effects of this magnitude *should* be described by a nonrelativistic theory encompassing Pauli paramagnetism. For a similar relativistic system of anomalous magnetic moments the free-particle energies for particles moving in the direction of the field are given by[4]

$$E^2 = m^2c^4 + c^2p^2 + \mu_0^2 H^2 + 2S\mu_0 Hmc^2 \tag{4}$$

where $S = \pm 1$. In the nonrelativistic limit, where all energies are small compared with mc^2, we find that

$$E \simeq (mc^2 + S\mu_0 H + p^2/2m)(1 + \mu_0^2 H^2/m^2c^4)^{1/2} \tag{5}$$

That is, the usual nonrelativistic energy levels are valid regardless of the relative magnitudes of $\mu_0 H$ and E_F, as long as both are much less than mc^2.

In the following discussion we shall demonstrate that the nonrelativistic theory of paramagnetism is capable of accomodating large fields after all, but only after formulating the mathematical description correctly. At the same time the analysis provides additional support for the efficacy of a method discussed earlier in connection with quantum statistical calculations[5,6].

2. PARAMAGNETISM IN THE BOLTZMANN LIMIT

At high temperatures and low densities the problem formulated above is completely described by the Boltzmann partition function for N particles in volume Ω,

$$Z_B(\beta,H) = \frac{1}{N!}\left[Z_1(\beta,H)\right]^N \tag{6}$$

in terms of the single-particle partition function[7]

$$\Omega^{-1} Z_1(\beta,H) = 2\lambda_T^{-3}\cosh(\beta\mu_0 H) \tag{7}$$

From the free energy $F = kT \ln Z_B$ one obtains the expected magnetic moment

$$\langle m\rangle = -\partial_H F = N\mu_0 \tanh(\beta\mu_0 H) \tag{8}$$

and when $\beta\mu_0 H \ll 1$

$$M \simeq n\mu_0^2 \beta H\ , \quad \chi \simeq n\mu_0^2\beta \tag{9}$$

There is no difficulty in this classical regime when the field strength is increased arbitrarily, for if $\beta\mu_0 H \gg 1$ we obtain immediately

$$M \simeq n\mu_0\left[1 - 2e^{-2\beta\mu_0 H}\right] \tag{10a}$$

$$\chi \simeq 4n\mu_0^2\beta e^{-2\beta\mu_0 H} \tag{10b}$$

That is, as H becomes very large the system saturates and the susceptibility tends to zero, exhibiting the maximum response. Moreover, this transition occurs smoothly, in agreement with our intuitive expectation that there will always be a few spins down as long as the field is finite. One should expect the mathematical and physical descriptions at low temperatures to be at least as satisfying.

3. THE DEGENERATE SYSTEM

We have shown in some detail elsewhere[6] that the grand potential, $f = \Omega^{-1} \ln Z_G$, can generally be written for non-interacting particles as a Mellin transform of the single-particle partition function, Eq. (7):

$$f = -i\, \lambda_T^{-3} \int_{c-i\infty}^{c+i\infty} t^{-5/2} e^{\beta\mu t} \csc(\pi t) \cosh(\beta\mu_0 H t)\, dt \ , \qquad 0 < c < 1 \qquad (11)$$

The number density is then given by $n = \beta^{-1} \partial_\mu f$, and the magnetization by $M = \beta^{-1} \partial_H f$. It will be more convenient in what follows to rewrite Eq. (11) in the form

$$\lambda_T^3 f = I(\alpha_+) + I(\alpha_-) \quad , \ \alpha_\pm = \beta(\mu \pm \mu_0 H) \qquad (12)$$

where

$$I(\alpha) = \frac{1}{2i} \int_{c-i\infty}^{c+i\infty} t^{-5/2}\, e^{\alpha t} \csc(\pi t)\, dt, \quad 0 < c < 1 \qquad (13)$$

and $\beta\mu \gg 1$ in the degenerate system. The integral converges for all real α.

When $\alpha \gg 1$ the contour can be closed to the left in a semicircle of radius R, with appropriate indentation to exclude the branch cut along the entire negative real axis. As R increases without bound the contributions from the circular arcs vanish, and, because there are no singularities contained within the closed contour, the only contribution to $I(\alpha)$ comes from the loop integral γ around the branch cut. That is,

$$I(\alpha) = -\frac{1}{2i} \int_\gamma t^{-5/2} e^{\alpha t} \csc(\pi t)\, dt \qquad (14)$$

where γ begins at $-\infty + i\varepsilon$, encircles the origin once in the negative direction, and returns to $-\infty - i\varepsilon$. The exponential cuts off the integrand at any significant distance from the origin in the left half--plane when $\alpha \gg 1$. Therefore $\csc(\pi t)$ can be expanded about the origin and term-by-term integration carried out by means of Hankel's integral formula for the Γ-function[8]

$$\frac{1}{\Gamma(z)} = -\frac{1}{2\pi i}\int_{\gamma} t^{-z} e^{t}\, dt \qquad (15)$$

The result is the asymptotic expansion

$$I(\alpha) = \pi\alpha^{3/2}\left[\frac{8}{15\pi^{3/2}}\alpha + \frac{\pi^{1/2}}{3\alpha} + O(\alpha^{-3})\right], \quad \alpha>>1 \qquad (16)$$

When $\beta\mu_0 H << 1$ this expansion can be used in both terms of Eq. (12) and one immediately regains the standard results of Eqs. (1)-(3). Although this expansion is always valid for evaluation of $I(\alpha_+)$, we see that it can not be employed for $I(\alpha_-)$, and hence for n_-, if α_- is small or negative. Thus, for large fields the integrals $I(\alpha_\pm)$, corresponding to spin-up and spin-down particles, respectively, must be evaluated separately.

We consider three separate regions for the evaluation of $I(\alpha_-)$. When $\alpha_- >> 0$ the expansion (16) is valid. If $\alpha_- \leqslant 0$ the contour in Eq. (13) can no longer be closed to the leff, but must now be closed in a semicircle to the right. The semicircular arc is chosen to pass between the poles of the integrand at $t = n$ and, whentheradlus increases without bound in discrete steps, the contribution from this arc vanishes. The integral is then evaluated by means of the residue theorem and one finds that

$$I(\alpha_-) = -\sum_{n=1}^{\infty}\frac{(-1)^n}{n^{5/2}}e^{-|\alpha_-|n} \qquad \alpha_- \leqslant 0 \qquad (17)$$

The series is uniformly and absolutely convergent for all α_-.

Despite the fact that the series expansion (17) was derived for non-positive values of a-, it can be analytically continued to small positive values as well. It is valid to take the term-by-term Mellin transform of the series (17) to obtain[9]

$$\begin{aligned} M(s) &= -\Gamma(s)\sum_{n=1}^{\infty}\frac{(-1)^n}{n^{s+5/2}} \\ &= (1-2^{-s-3/2})\,\zeta(s+5/2)\Gamma(s)\,, \quad \mathrm{Re}(s) > 0 \end{aligned} \qquad (18)$$

where in the second line we have used a well-known identity for the generalized Riemann zeta-function[10]. Now perform the inverse Mellin transformation. As usual, this is evaluated by closing the Mellin contour to the left and employing the known asymptotic properties of $\Gamma(s)$ and $\zeta(s)$ on the semicircular arc[11]. The contribution from this arc vanishes and the integral is given by the sum of the residues at the poles of the Γ-function: $s = -n$ with residue $(-1)^n/n!$. Note that the single simple pole of $\zeta(z)$ at $z = 1$ is cancelled by the factor multiplying the function $\zeta(s+5/2)$ in Eq. (18). Therefore,

$$I(\alpha_-) = \sum_{n=0}^{\infty} \frac{\alpha_-^n}{n!} \zeta(5/2-n)(1-2^{n-3/2}) \ , \quad \alpha_- \geqslant 0 \tag{19}$$

which converges absolutely for $|\alpha_-| < \pi$ and is regular within this circle. Observe that the two expressions (17) and (19) join smoothly at $\alpha_- = 0$, because at this point both reduce to

$$I(0) = (1-8^{-1/2})\zeta(5/2) \tag{20}$$

A similar method of analytic continuation was employed by Robinson[12] to study the Bose-Einstein integrals, but the resuls are completely different owing to the alternating signs in Eq. (17).

Now it is possible to characterize the spin-down integral in the physical regions of interest for various values of the magnetic field strength:

$$\begin{aligned} I(\alpha_-) &= \pi\alpha_-^{3/2} \left[(8/15\ \pi^{3/2})\alpha_- + (\pi^{1/2}/3)\alpha_-^{-1} + O(\alpha_-^{-3})\right] \ , \quad \alpha_- \gg 1 \\ &= \sum_{n=0}^{\infty} \frac{\alpha_-^n}{n!} \zeta(5/2-n)(1-2^{n-3/2}) \ , \quad -1 < \alpha_- < 1 \\ &= -\sum_{n=1}^{\infty} \frac{(-1)^n}{n^{5/2}} e^{-|\alpha_-|n} \ , \quad \alpha_- < -1 \\ &\xrightarrow[\alpha_- \ll -1]{} e^{-|\alpha_-|} \end{aligned} \tag{21}$$

and the spin-up integral $I(\alpha_+)$ is always given by Eq. (16). Although the nature of the finite-temperature corrections is now obvious within each region, we shall consider only the terms contributing at zero temperature. In this limit the number density $n = n_+ + n_-$ is given by

$$n_+ = 4\alpha_+^{3/2}/3\pi^{1/2}\lambda_T^3 \tag{22a}$$

$$\begin{aligned} n_- &= 4\alpha_-^{3/2}/3\pi^{1/2}\lambda_T^3 \quad , \quad \alpha_- \gg 1 \\ &= \zeta(3/2)(1-2^{-1/2})\ \lambda_T^{-3} \quad , \quad -1 < \alpha_- < 1 \\ &= e^{-|\alpha_-|} \quad , \quad \alpha_- \ll -1 \end{aligned} \tag{22b}$$

and the magnetization follows from Eq. (1).

The degenerate Fermi gas of charge-neutral, spin-1/2 particles can now be described over the full range of magnetic field strengths. As the field increases, n_- decreases smoothly to a small value at $\mu = \mu_0 H$. In this region it contributes essentially nothing to n, because $n_- = 0(k^3T^3)$. As H is increased further, n_- falls off exponentially, as expected, and the system saturates with the magnetic susceptibility vanishing smoothly as $T \to 0$ and $H \to \infty$. This provides a completely satisfactory description for all field strengths, both physically and mathematically.

In the high-field region the chemical potential is readily evaluated in terms of the density

$$n \simeq n_+ \simeq (4\beta^{3/2}/3\pi^{1/2}\ \lambda_T^3)(\mu+\mu_0 H)^{3/2} \tag{23}$$

which can not depend on the field. As $T \to 0$ we have $\mu(T=0) = E_F$(H), or

$$\mu(T=0) = 2^{2/3}E_F(H=0) - \mu_0 H \ . \tag{24}$$

Large magnetic fields will reduce the effective Fermi energy and, for electrons in fields on the order of 10^9 G, $E_F(H)$ will pass through zero and take on negative values. This phenomenon does not appear to be experimentally accessible at this time.

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Resumo

A magnetização de um gás ideal de férmions com momentos magnéticos é reexaminada. Para campos magnéticos externos muito intensos a magnetização é representada de uma maneira que e, fisicamente e matematicamente, completamente satisfatória.