Peierls' Elucidation of Diamagnetism

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This article summarizes the contribution to the phenomenon of Diamagnetism made by Rudolf Peierls, as Quantum Mechanics was triumphantly unfolding in the 1930's.

For a macroscopic system to which Statistical Mechanics applies, the boundary contribution to physical attributes is not expected to be significant. This is because for an N-particle system, the ratio of the boundary-to-bulk particles scales as $N^{-1/3}$, which is vanishingly small when N is very large. Be that as it may, when it comes to diamagnetism, the boundary does matter, and this is why Peierls ascribed to diamagnetism the epithet of 'Surprises in Theoretical Physics' [1].

Diamagnetism, or the response to an applied magnetic field of the orbital motion of a collection of charged particles, is quantified by the magnetization vector written as

$$\mathbf{M} = \frac{eN}{2mc}\langle \mathbf{L} \rangle \, , \tag{1}$$

where the angular brackets $\langle - \rangle$ imply a statistical average, e is the electric charge, m is the mass of the particle, c is the speed of light and the angular momentum operator $\mathbf{L}$ is defined by

$$\mathbf{L} = \mathbf{r} \times \mathbf{P}_{\text{kin}} \, . \tag{2}$$

In the above $\mathbf{r}$ is the position operator of the particle while $\mathbf{P}_{\text{kin}}$ is what is called the 'kinematic' momentum, and the important point of Electrodynamics is that $\mathbf{P}_{\text{kin}}$ differs from the 'canonical' momentum $\mathbf{p}$ by the presence of the vector potential $\mathbf{A}$:

$$\mathbf{P}_{\text{kin}} = \left(\mathbf{p} - \frac{e\mathbf{A}}{c} \right) \, . \tag{3}$$

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It is through $\mathbf{A}$ that the magnetic field $\mathbf{B}$ enters into the discussion via the relation:

$$\mathbf{B} = \text{Curl } \mathbf{A} \,. \tag{4}$$

Combining (1)–(3) we arrive at

$$\mathbf{M} = \frac{eN}{2c} \langle (\mathbf{rxv}) \rangle \,, \tag{5}$$

where the velocity operator has its 'mechanistic' definition of

$$\mathbf{v} = \frac{\mathbf{P}_{\text{kin}}}{m} \,. \tag{6}$$

Equation (5) makes Peierls' argument clear: while the number of electrons in a material on the boundary is indeed small, a substantial portion of the boundary electrons has however a large contribution to $\mathbf{M}$ because of the largeness of the magnitude of the position vector $\mathbf{r}$ when the origin of the coordinate system is fixed once and for all. It is this boundary contribution that exactly nullifies the bulk contribution to $\mathbf{M}$ in classical statistical mechanics, leading to the celebrated Bohr–van Leeuwen theorem which states that *Diamagnetism does not exist in Classical Mechanics* [2]! Did Bohr and van Leeuwen actually calculate the boundary contribution and show that it exactly cancels the bulk one? The answer is NO, and is clarified by another ingenious analysis of Peierls, as presented below.

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Note that (5) can be alternately expressed as

$$\mathbf{M} = -\left\langle \frac{\partial H}{\partial \mathbf{B}} \right\rangle \,, \tag{7}$$

where H is the Hamiltonian for an N-particle system

$$H = \frac{1}{2m} \sum_{i=1}^{N} \left(\mathbf{p}_i - \frac{e\mathbf{A}_i}{c} \right)^2 \,. \tag{8}$$

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This then allows a calculation of $\mathbf{M}$ through the canonical partition function Z:

$$\mathbf{M} = k_{\mathrm{B}} T \frac{\partial}{\partial \mathbf{B}} \ln Z\,, \tag{9}$$

where k_{B} is the Boltzmann constant, T is the temperature and $\ln Z$ defines the logarithm of the partition function. Peierls and van Vleck [3] demonstrated that while calculation via (7) is extremely sensitive to the boundary conditions, that through the partition function route of (9) is not! Because the partition function in classical statistical mechanics involves an integral over the entire phase space of position and momentum variables, the dependence of Z on $\mathbf{B}$ disappears upon a change of integration variables and therefore the derivative (with respect to $\mathbf{B}$ as in (9)) vanishes.

Of course, a real material such as bismuth (Bi) does exhibit diamagnetism and quantum mechanics comes to the rescue through the brilliant work of Landau [4]. Landau, as Peierls has shown in [1], preferred to do his calculation through (9), and arrived at the following answer (for non-degenerate electrons for which the Fermi–Dirac statistics is not crucial):

$$M = -\frac{N k_{\mathrm{B}} T}{B} \left[\frac{B\mu_{\mathbf{B}}}{k_{\mathrm{B}} T} \coth\left(\frac{B\mu_{\mathrm{B}}}{k_{\mathrm{B}} T}\right) - 1 \right], \tag{10}$$

It is evident that in the appropriate classical limit (of the Planck constant $\hbar \to$ 0 and $T \to \infty$, $\mathbf{M}$ does reduce to zero, in agreement with the Bohr–van Leeuwen theorem.

$\mu_{\mathrm{B}} (= e\hbar/2mc)$ being the Bohr magneton. In Equation (10) we have removed the boldface on $\mathbf{M}$ and considered only the component along the $\mathbf{B}$ field. It is evident that in the appropriate classical limit (of the Planck constant $\hbar \to 0$ and $T \to \infty$), $\mathbf{M}$ does reduce to zero, in agreement with the Bohr–van Leeuwen theorem. This then establishes diamagnetism as a quintessential quantum property and also demonstrates, *a la* Landau and Peierls, that the cancellation of the bulk contribution by the boundary one is incomplete in quantum mechanics. Today the boundary contribution to M, captured by the so-called 'Edge Currents', has acquired great significance in the discussion of the Quantum Hall Effect [5]. One other newer initiative in the Peierls analysis of diamagnetism is in the context of quantum dissipation [6]. The issue is: Because boundary effects are critical for diamagnetism and are also a ubiquitous ingredient of the topically important nano-systems, what influence does dissipation have on diamagnetism? The question is crucially relevant for a nano-system as the latter is invariably under the non-negligible and noisy influence of the environment. The analysis has led to the understanding of the dissipation induced transition from the Landau to the Bohr–van Leeuwen regimes [7], the unification of the Gibbs and Einstein approaches to Statistical mechanics [8] and also the clarification of the low-temperature thermodynamics in relation to the third law [9].

Because boundary effects are critical for diamagnetism and are also a ubiquitous ingredient of the topically important nano-systems, what influence does dissipation have on diamagnetism?

The above treatment of diamagnetism, as has been stated already, is restricted to non-degenerate electrons which, though handled quantum mechanically, are assumed to obey the Boltzmann statistics. Peierls however did consider also the realistic property of metals at low temperatures to which the Fermi–Dirac statistics apply. The result was a beautiful illustration of a novel oscillating behavior of the low-temperature diamagnetism as a function of the magnetic field [10]. The analysis runs as follows.

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In the presence of a magnetic field B the energy eigenvalues of the Hamiltonian in (8) are distributed in discrete Landau levels. Each level is however highly degenerate. The degeneracy G, i.e., the number of quantum states associated with a given level, say the ground level, is given by:

$$G = \frac{eBA}{2\pi\hbar c}\ , \tag{11}$$

where A is the area of the film to which the B-field is applied normally. This means that at $T = 0$, N electrons

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can be accommodated at the lowest Landau level (ignoring spin), provided that $N < G$. The corresponding diamagnetic moment is:

$$M = -N\mu_{\rm B}\,. \tag{12}$$

Now, if B is decreased such that G falls below N, $N-G$ electrons have to go to the next higher level. The total energy is then

$$E = B\mu_{\rm B}G + 3B\mu_{\rm B}(N-G) = 3NB\mu_{\rm B} - 2B\mu_{\rm B}G\,. \tag{13}$$

Correspondingly

$$M = -\frac{\partial E}{\partial B} = -3N\mu_{\rm B} + 4G\mu_{\rm B}\,. \tag{14}$$

Equation (14) is key to the phenomenon of oscillation. Note that tuning the magnetic field is tantamount to tuning the degeneracy factor G. If all the electrons are accommodated in the lowest level, $G = N$ and $M = N\mu_{\rm B}$. On the other hand, if only the first two levels are fully occupied and all the higher levels are empty, then $G = \frac{N}{2}$ and $M = -N\mu_{\rm B}$, indicating a switch in the sign of the magnetization. This elegant and simple analysis of the diamagnetic oscillation by Peierls had been seen experimentally in Bi by de Haas and van Alphen [11], comprehensively reviewed by Shoenberg [12].

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