On Non-zero Classical Diamagnetism: A Surprise

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It is well known that the orbital diamagnetism of a classical system of charged particles in thermal equilibrium is identically zero – the Bohr-van Leeuwen theorem. Physically, this null result derives from the exact cancellation of the orbital diamagnetic moment associated with the complete cyclotron orbits of the charged particles by the paramagnetic moment subtended by the incomplete orbits skipping the boundary in the opposite sense. Motivated by this crucial, but subtle role of the boundary, we have considered here the case of a finite but *unbounded* system, namely that of a charged particle moving on a sphere in the presence of an externally applied magnetic field. The calculated moment now indeed turns out to be non-zero, and has the diamagnetic sign. To the best of our knowledge, this is the first report of the possibility of finite classical diamagnetism, and it is due to the avoided cancellation. Possible experimental realization is discussed.

In this work we re-visit the problem of the absence of classical diamagnetism of a system of charged particles in thermal equilibrium. This vanishing of the classical diamagnetism in equilibrium is generally referred to as the Bohr-van Leeuwen theorem [1, 2, 3, 4]. The fact that classically the orbital diamagnetic moment vanishes is quite contrary to our physical expectations inasmuch as a charged particle (of charge $-e$, position $\mathbf{r}(t)$, and velocity $\mathbf{v}(t)$ at time t), say, orbiting in a plane perpendicular to the magnetic field $\mathbf{B}$ under its Lorentz force should have an orbital magnetic moment $\mathbf{M}\,(= -e/2c\big[\mathbf{r}(t)\times\mathbf{v}(t)\big])$, where c is the speed of light, and with a diamagnetic sign as dictated by the Lenz's law (see e.g. [5]).

The vanishing of the classical diamagnetism is due, however, to a subtle role played by the boundary of the finite sample. It turns out that the diamagnetic contribution of the completed cyclotron orbits of the charged particles orbiting around the magnetic field in a plane perpendicular to it, is cancelled by the paramagnetic contribution of the incomplete orbits skipping the boundary in the opposite sense in a cuspidal manner. The cancellation is exact, and that is the surprise. This cancellation was demonstrated explicitly some time back [6] for the case of a harmonic-potential ($V(r) = kr^2/2$) confinement, which is equivalent to a soft boundary, and finally letting the spring constant k go to zero. The treatment was based on the classical Langevin equation [7], and the magnetic moment $\mathbf{M} = -e/2c\big[\mathbf{r}(t)\times\mathbf{v}(t)\big]$ was calculated in the infinte-time limit – the Einsteinien approach to statistical mechanics. The ordering of the two limits namely $k \to 0$ (the deconfinement limit) and $t \to \infty$ (the infinite time limit), however, turned out to be crucial and physically meaningful – one must let $t \to \infty$ first and then let $k \to 0$. This ensures that the particle is affected by the boundary, or the confinement. Thus one had to conclude that any orbital diamagnetism observed in an experiment is essentially of quantum-mechanical origin, as indeed was derived first by Landau [8]. In the quantum case, the above cancelllation of the bulk and the boundary contributions turns out to be incomplete. But again, the order of the two limits is all important and was implicit in the treatment of Landau [3]. It was shown more explicitly by Darwin [9]. In fact, one could just use the quantum Langevin equation [10] and derive essentially the Landau result by properly taking the above 'Darwin limit'. The calculated diamagnetic moment is found to depend on the frictional term occuring in the quantum Langevin equation [11, 12].

The subtle but essential role of the boundary in all these treatments has motivated us to examine the diamagnetism for a classical system that has no geometrical boundary – a finite *unbounded* system such as a charged particle moving on the surface of a sphere under the appropriate Langevin dynamics in the presence of an external magnetic field. We were pleasantly surprised to find that the numerically calculated orbital magnetic moment turned out to be nonzero, and indeed diamagnetic. To the best of our knowledge, this is the first example reported on nonzero orbital diamagnetism for a classical system. It arises explicitly from avoided cancellation as the system has no boundary.

Consider a charged particle (charge -e and mass m, an electron say) moving on the surface of a sphere of radius 'a', in the presence of a uniform externally applied magnetic field $\mathbf{B}$ directed along the $z-$axis. The particle motion is described by the following classical Langevin equation

$$m\frac{d\mathbf{v}}{dt} = -\frac{e}{c}(\mathbf{v}\times\mathbf{B}) - \Gamma\mathbf{v} + \sqrt{2\Gamma k_B T}\,\mathbf{f}(t) \qquad (1)$$

where Γ is the friction coefficient, k_BT the thermal energy, and $\mathbf{f}$ is a zero-mean $\delta-$correlated Gaussian random noise, i.e., $\langle f_\alpha(t) f_\beta(t')\rangle = \delta_{\alpha\beta}\delta(t-t')$. We recall here that in this real space-time (Einsteinian) approach to statistical mechanics, the long-time limit ($t \to \infty$) of the above stochastic evolution gives the thermal-equilibrium properties.

Specializing now to the spherical-polar coordinates appropriate to the motion on the surface of the sphere $(r = a, \theta, \phi)$, the Langevin equation reduces to

$$a\Big[\frac{d^2\theta}{dt^2} - \sin\theta\cos\theta\,\big(\frac{d\phi}{dt}\big)^2\Big]\,\hat{\boldsymbol{\theta}} + a\Big[\sin\theta\,\frac{d^2\phi}{dt^2} + 2\,\cos\theta\,\frac{d\theta}{dt}\,\frac{d\phi}{dt}\Big]\,\hat{\boldsymbol{\phi}} \;=\; -\frac{eB}{mc}\,a\,\Big[\frac{d\theta}{dt}\,\hat{\boldsymbol{\theta}} + \sin\theta\,\frac{d\phi}{dt}\,\hat{\boldsymbol{\phi}}\Big] \times (\hat{\mathbf{r}}\,\cos\theta)$$
$$-\frac{a\Gamma}{m}\Big[\frac{d\theta}{dt}\,\hat{\boldsymbol{\theta}} + \sin\theta\,\frac{d\phi}{dt}\,\hat{\boldsymbol{\phi}}\Big] + \frac{\sqrt{2\Gamma k_B T}}{m}\Big(f_\theta\,\hat{\boldsymbol{\theta}} + f_\phi\,\hat{\boldsymbol{\phi}}\Big), \tag{2}$$

where $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ are the unit vectors directed along the radial (r), polar (θ) and the azimuthal (ϕ) directions. Also, f_θ and f_ϕ are the forcing noise terms acting along the θ and the ϕ directions respectively. More conveniently, we re-write equation (2) in the dimensionless form

$$\ddot{\theta} - \sin\theta\cos\theta\dot{\phi}^2 \;=\; -\frac{\omega_c}{\gamma}\sin\theta\cos\theta\dot{\phi} - \dot{\theta} + \sqrt{\eta}f_\theta \tag{3a}$$
$$\sin\theta\ddot{\phi} + 2\cos\theta\dot{\theta}\dot{\phi} \;=\; \frac{\omega_c}{\gamma}\cos\theta\dot{\theta} - \sin\theta\dot{\phi} + \sqrt{\eta}f_\phi, \tag{3b}$$

where we have introduced the cyclotron frequency $\omega_c = eB/mc$, the frictional velocity relaxation rate $\gamma = \Gamma/m$, the thermal forcing strength $\eta = 2k_BT/(ma^2\gamma^2)$, and the dimensionless time $\tau = \gamma t$. Note that η is also a dimensionless quantity. Here overhead dots denote differentiation with respect to the dimensionless time τ. The physical quantity of interest is the ensemble averaged orbital magnetic moment

$$\langle M(\tau)\rangle = -\frac{e}{2c}\,\gamma\,a^2\langle\sin^2\theta(\tau)\dot{\phi}(\tau)\rangle \tag{4}$$

in the long-time limit, where $\langle\cdots\rangle$ denotes the ensemble average over the different realizations of the stochastic forces f_θ and f_ϕ.

We now rewrite the above second-order differential Langevin equations (3) as four coupled first-order equations for θ, $x\,(\equiv\dot{\theta})$, ϕ, and $y\,(\equiv\dot{\phi})$, which are then solved numerically using a simple Euler-Maruyama scheme [13] with a time-step $\Delta\tau = 10^{-2}$. Averages are evaluated over $n = 10^6$ noise realizations. The number of realizations, though quite large, is necessarily finite, and so we resort to double average $\langle\langle\cdots\rangle\rangle$ denoting averaging over the ensemble as well as over time. This gives for the equilibrium magnetic moment

$$M_{eq} = \langle\langle M(\tau)\rangle\rangle \equiv \frac{1}{\tau_{max}}\int_0^{\tau_{max}}\langle M(\tau)\rangle\,d\tau \tag{5}$$

as $\tau_{max}\to\infty$. In the context of numerical simulation, we have to be careful at the singular polar points $\theta = 0$ and $\theta = \pi$, where $1/\sin\theta$ diverges. This is regularized by replacing $\sin\theta$ by $\sqrt{\sin^2\theta + \epsilon}$ where ϵ is a small positive quantity taken to be of order $\Delta\tau$. Further, inasmuch as the physical motion is restricted to $0 \le \theta < \pi$ and $0 \le \phi < 2\pi$, while mathematically, however, the equations (3) can evolve outside these bounds, we have to set in our numerical simulation the following conditions: If $\theta(\tau) < 0$, then $\theta(\tau) \to -\theta(\tau)$, $x(\tau) \to -x(\tau)$, $\phi(\tau) \to \phi(\tau - \Delta\tau) + \pi$; and if $\theta(\tau) > \pi$, then $\theta(\tau) \to 2\pi - \theta(\tau)$, $x(\tau) \to -x(\tau)$, $\phi(\tau) \to \phi(\tau - \Delta\tau) - \pi$. This takes care of the trajectories that happen to pass through the poles. The choice of initial conditions on θ and ϕ, and their time derivatives, turns out to be irrelevant for the long-time ensemble averaged behavior as indeed is validated by our numerical simulation.

In FIG. 1, we have plotted the dimensionless magnetic moment $\langle\mu(\tau)\rangle = 2c/(e\gamma a^2)\,\langle M(\tau)\rangle$ as a function of τ for certain choice of ω_c/γ and η. As can be readily seen, the moment is diamagnetic and odd in the magnetic field. Also, it can shown to be independent of the sign of the charge (electron or hole) as indeed it must be. The fluctuations seen in the figure are statistical fluctuations due to the finiteness of the number of realizations used for ensemble averaging. These are thus statistical fluctuations – these will, and indeed do, decrease with increasing number of noise realizations n.

FIG. 2 shows the variation of the dimensionless magnetic moment μ_{eq} (corresponding to M_{eq}) with the magnetic field ω_c/γ (which is proportional to $\mathbf{B}$). The plot shows an essential linear response which is diamagnetic.

Finally in FIG. 3, we have plotted the probability density $P(\mu)$ of the statistical mechanical fluctuations about the equilibrium value μ_{eq}. The distribution for the chosen values of the parameters is quite broad relative to the mean. (The corresponding plot for a system *with* a boundary is indeed known to be broad [14]. Of course, in that case the mean is zero.)

It will be apt at this stage to make a few comments. First, we recall that the nonzero diamagnetic moment for the classical system discussed above is due entirely to the absence of a boundary – the avoided cancellation for a finite but *unbounded* system. Now, for the case of the quantum mechanical (Landau) diamagnetism too there is a cancellation, but it is incomplete [3]. Hence the smallness of the Landau diamagnetism in general. We may reasonably expect then that the quantum mechanical diamagnetism for a finite but unbounded system too should be much larger because of the avoided cancellation

[15]. Second, the finite but unbounded system considered in this work is physically realizable. Thus, we could consider a dielectric microsphere coated with an ultrathin layer of a conducting material having small carrier concentration at room temperature, e.g., a non-degenerate system with the degeneracy temperature much smaller than the room temperature, as in the case of a doped high-mobility semiconductor. (By ultrathin we mean here a thickness $\ll$ the thermal de Broglie wavelength of charge carriers so as to freeze out the radial motion, making the system essentially a two-dimensional classical gas of charged particles). We could indeed consider a finite volume fraction of an inert medium (paraffin say) occupied by the above microspheres. This system should have a measurable diamagnetic response. Third, it should be interesting to consider more general geometries such as that of a triaxial ellipsoid where different axes ratios can mimick very different physical situations. Perhaps much more interesting will be to try out topologies other than that of a sphere and look for qualitative differences [15]. Finally, the numerical value of the diamagnetic moment of a charged particle (say, electron) moving on a sphere of radius $a = 100\mu m$ for $B \simeq 5$ kilogauss, $\gamma \sim 10^9 s^{-1}$ turns out to be ~ 5 Bohr magnetons per electron per gauss. Compare this with the Landau diamagnetic moment *per electron* per gauss for Bismuth which is known to have one of the highest diamagnetic susceptibility of about 10^{-4} cgs units [16]. The calculated value turns out to be $\simeq 10^{-7}$ Bohr magnetons per electron per gauss, where we have assumed the electron number density to be $\sim 10^{23} cm^{-3}$. Thus, on the per electron per gauss basis, the classical orbital diamagnetism in the case considered here is orders of magnitude larger than that for one of the highest values of Landau diamagnetism known in normal metals/semimetals – we have a giant classical diamagnetism. Of course, the measured bulk susceptibility for the physical classical system suggested above may have much smaller values because of the parameter values realized. But, the point of principle at issue will have been made.

To conclude, we have shown that a classical system of charged particles moving on a finite but *unbounded* surface (of a sphere) has a nonzero orbital diamagnetic moment which can be large. This is a surprise.

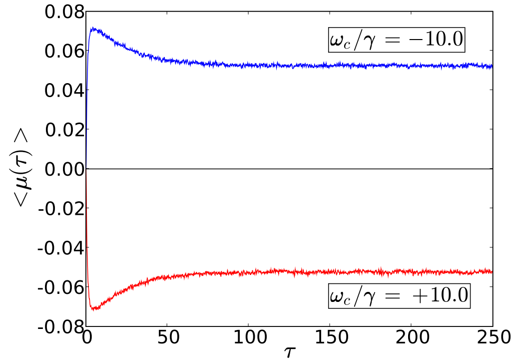

FIG. 1: (Color online) Plot of the ensemble averaged dimensionless magnetic moment $\mu(\tau)$ as a function of the dimensionlesss time τ for $\omega_c/\gamma = \pm 10.0$ and $\eta = 1.0$. Clearly the moment can be seen to be odd in the magnetic field **B** and is diamagnetic.

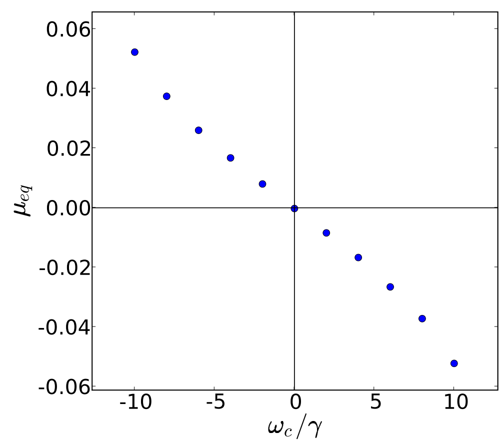

FIG. 2: (Color online) Plot of the dimensionless magnetic moment μ_{eq} as a function of ω_c/γ (proportional to the magnetic field) for $\eta = 1.0$. Again the moment is found to be odd in **B** and is diamagnetic in sign.

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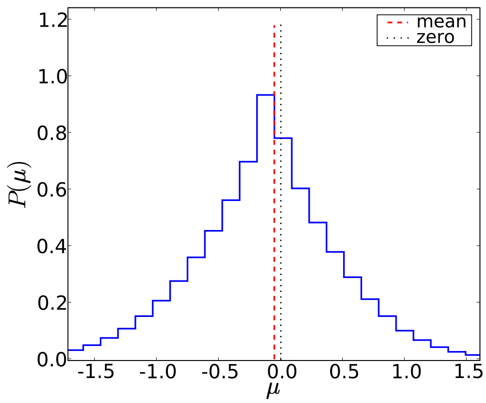

FIG. 3: (Color online) Plot of the long-time probability density $P(\mu)$ against μ giving the ensemble fluctuations about μ_{eq}. The latter is clearly nonzero and diamagnetic. The fluctuations are seen to be large compared to the mean value. Here $\omega_c/\gamma = 10.0$ and $\eta = 1.0$.

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