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Classical Langevin dynamics of a charged particle moving on a sphere and diamagnetism: A surprise

N. Kumar[1,3(a)] and K. Vijay Kumar[2(b)]

[1] *Raman Research Institute - Bangalore 560 080, India*
[2] *CCMT, Department of Physics, Indian Institute of Science - Bangalore 560 012, India*
[3] *Jawaharlal Nehru Centre for Advanced Scientific Research - Bangalore 560 064, India*

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Abstract – It is generally 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 simulated here the case of a finite but *unbounded* system, namely that of a charged particle moving on the surface of a sphere in the presence of an externally applied uniform magnetic field. Following a real space-time approach based on the classical Langevin equation, we have computed the orbital magnetic moment that 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 in principle, and it is due to the avoided cancellation.

In this work, we revisit 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 [1–4]. 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 $\mathbf{M}\,(=-e/2c[\mathbf{r}(t)\times\mathbf{v}(t)])$, where c is the speed of light, and with a diamagnetic sign as dictated by Lenz's law (see, *e.g.*, [5]). Formally, the vanishing of the classical diamagnetic moment follows from the well-known fact that the canonical partition function involves the Hamiltonian for the charged particle (coupled minimally to the static magnetic field) and a simple shift of the canonical momentum variable in the integration makes the partition function field-independent, giving zero magnetic moment [3].

Physically, the vanishing of the classical diamagnetism is due, however, to a subtle role played by the boundary of the finite sample [1–4]. 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 $\mathbf{M}=-e/2c[\mathbf{r}(t)\times\mathbf{v}(t)]$ was calculated in the infinite-time limit —the Einsteinian 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

(a) E-mail: nkumar@rri.res.in
(b) E-mail: vijayk@physics.iisc.ernet.in

experiment is essentially of quantum-mechanical origin, as indeed was derived first by Landau [8]. In the quantum case, the above cancellation 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]. This 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, however, 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 a uniform external magnetic field. We were pleasantly surprised to find that the numerically computed orbital magnetic moment turned out to be non-zero, and indeed diamagnetic. To the best of our knowledge, this is the first example reported on non-zero orbital diamagnetism in principle 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

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

where Γ is the friction coefficient, $k_{\mathrm{B}}T$ is the thermal energy, and $\mathbf{f}$ is a zero-mean δ-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 is expected to give the thermal-equilibrium properties. Note that there is no modification of the dissipation (Γ) and the related noise term $(\mathbf{f}(t))$ due to the magnetic field [7].

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

$$\begin{aligned}
& a\left[\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} - \sin\theta\cos\theta\left(\frac{\mathrm{d}\phi}{\mathrm{d}t}\right)^2\right]\hat{\boldsymbol{\theta}} \\
& + a\left[\sin\theta\,\frac{\mathrm{d}^2\phi}{\mathrm{d}t^2} + 2\,\cos\theta\,\frac{\mathrm{d}\theta}{\mathrm{d}t}\,\frac{\mathrm{d}\phi}{\mathrm{d}t}\right]\hat{\boldsymbol{\phi}} = \\
& \quad -\frac{eB}{mc}\,a\left[\frac{\mathrm{d}\theta}{\mathrm{d}t}\,\hat{\boldsymbol{\theta}} + \sin\theta\,\frac{\mathrm{d}\phi}{\mathrm{d}t}\,\hat{\boldsymbol{\phi}}\right]\times(\hat{\mathbf{r}}\,\cos\theta) \\
& \quad -\frac{a\Gamma}{m}\left[\frac{\mathrm{d}\theta}{\mathrm{d}t}\,\hat{\boldsymbol{\theta}} + \sin\theta\,\frac{\mathrm{d}\phi}{\mathrm{d}t}\,\hat{\boldsymbol{\phi}}\right] + \frac{\sqrt{2\Gamma k_{\mathrm{B}}T}}{m}\left(f_\theta\,\hat{\boldsymbol{\theta}} + f_\phi\,\hat{\boldsymbol{\phi}}\right),
\end{aligned} \tag{2}$$

where $\hat{r}$, $\hat{\boldsymbol{\theta}}$ and $\hat{\phi}$ 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 eq. (2) in the dimensionless form

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

$$\sin\theta\ddot{\phi} + 2\cos\theta\dot{\theta}\dot{\phi} = \frac{\omega_c}{\gamma}\cos\theta\dot{\theta} - \sin\theta\dot{\phi} + \sqrt{\eta}f_\phi, \tag{4}$$

where we have introduced the cyclotron frequency $\omega_c = eB/mc$, the frictional velocity relaxation rate $\gamma = \Gamma/m$, the thermal forcing strength $\eta = 2k_{\mathrm{B}}T/(ma^2\gamma^2)$ 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

$$\langle M(\tau)\rangle = -\frac{e}{2c}\,\gamma\,a^2\langle\sin^2\theta(\tau)\dot{\phi}(\tau)\rangle \tag{5}$$

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 (4) 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

$$M_{\mathrm{eq}} = \langle\langle M(\tau)\rangle\rangle \equiv \frac{1}{\tau_{\max}}\int_0^{\tau_{\max}}\langle M(\tau)\rangle\,\mathrm{d}\tau \tag{6}$$

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 $0\leqslant\theta<\pi$ and $0\leqslant\phi<2\pi$, while mathematically, however, eqs. (3) and (4) 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

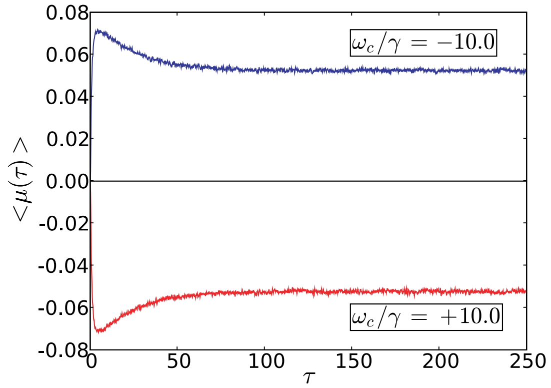

Fig. 1: (Colour on-line) Plot of the ensemble averaged dimensionless magnetic moment $\mu(\tau)$ as a function of the dimensionless time τ for $\omega_c/\gamma = \pm 10.0$ and $\eta = 1.0$. Clearly the moment can be seen to be odd in the magnetic field **B** and is diamagnetic.

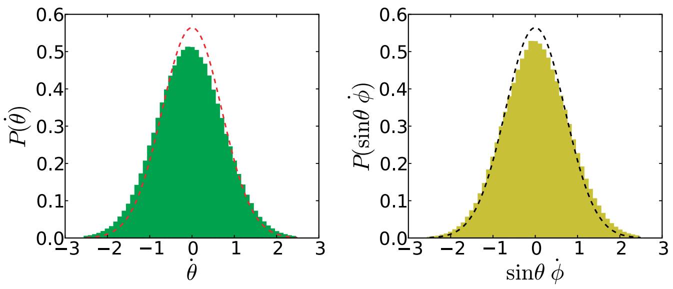

Fig. 2: (Colour on-line) The velocity distribution on a sphere in the presence of magnetic field computed from the Langevin dynamics simulation. The dashed curve is the corresponding Maxwellian distribution. Here, $\omega_c/\gamma = 10.0$ and $\eta = 1.0$.

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 be 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.

For completeness, we have also plotted the computed velocity distributions (the θ and ϕ components) in fig. 2 and these are seen to be essentially Maxwellian as expected, with the correct mean square values consistent with the fluctuation-dissipation theorem. In fact, there is no dependence on the external magnetic field.

Figure 3 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 **B**). The plot shows an essential linear response that is diamagnetic.

In fig. 4, 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

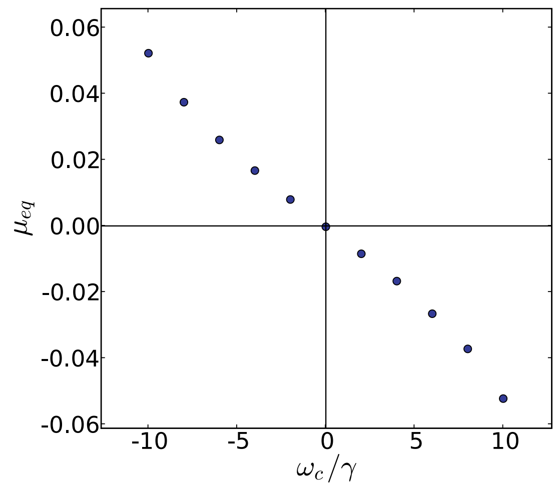

Fig. 3: (Colour on-line) Plot of the dimensionless magnetic moment μ_{eq} as a function of ω_c/γ (proportional to the magnetic field) for $\eta = 1.0$. Again, the moment is found to be odd in **B** and is diamagnetic in sign.

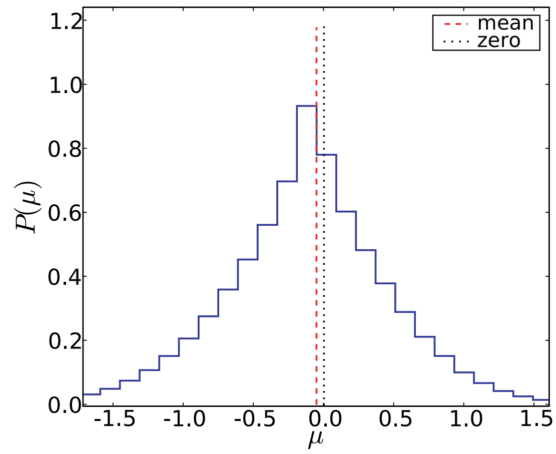

Fig. 4: (Colour on-line) Plot of the long-time probability density $P(\mu)$ against μ giving the ensemble fluctuations about μ_{eq}. The latter is clearly non-zero and diamagnetic. The fluctuations are seen to be large compared to the mean value. Here, $\omega_c/\gamma = 10.0$ and $\eta = 1.0$.

known to be broad [14]. Of course, in that case the mean is zero.)

We now return to the main point of this puzzle, namely that the classical Langevin dynamics for this finite unbounded system gives a non-zero diamagnetic moment, and yet a straightforward calculation using the canonical partition function with a minimally coupled Hamiltonian gives a free energy that is independent of the magnetic field, and therefore, a zero field-derivative of the latter implying zero diamagnetism. Now, the classical Langevin dynamics provides a real space-time picture of the charged particle motion under the influence of fluctuations and the concomitant dissipation. Its long-time limit is expected to describe thermal equilibrium, and sure enough it does reproduce the Maxwellian velocity distribution (fig. 2). Moreover, it is manifestly gauge-invariant because it involves the magnetic field directly without invoking a vector potential (indeed, in classical electrodynamics, the vector potential is essentially a matter of convenience, unlike in the case of quantum mechanics). Also, the computed diamagnetism is consistent with the Lenz's law. On the other hand, the canonical treatment based on the Hamiltonian underlies all of the classical statistical mechanics, but it gives zero classical diamagnetism. Our resolution of this puzzle is as follows: It is known that classically the static magnetic field does no work on the moving charge inasmuch as the Lorentz force $(-\frac{e}{c}(\mathbf{v}\times\mathbf{B}))$ acts perpendicular to the instantaneous velocity vector. However, such a gyroscopic force can still alter the motion of the charged particle so as to give a non-zero magnetic moment *without changing its energy.* In fact, it induces a correlation between the velocity and the transverse acceleration due to the Lorentz force. Clearly, such a subtle dynamical correlation, without change of energy, is not captured by the equilibrium partition function. But, the Langevin dynamics manifestly treats this gyroscopic Lorentz force through the equation of motion. It is thus our view that the real space-time treatment based on the Langevin dynamics takes into account these subtle correlations involving velocity and the transverse acceleration caused by the Lorentz force without changing the energy, which is missing from the usual partition function. Of course, this disagreement is only for the special case of a strictly unbounded classical system in an external magnetic field.

Thus, we are forced to admit that there are two alternatives —either there is indeed non-zero classical diamagnetism for an unbounded finite system as under consideration, or the classical Langevin dynamics fails to describe in the long-time limit the thermal equilibrium as described by the classical partition function in the presence of a magnetic field[1]. Either way, we have a non-trivial result.

Finally, it will be apt at this stage to make a few comments, bearing on the physical realizability of such a classical system.

First, we recall that the non-zero 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 different, probably larger, because of the avoided cancellation [15]. Second, our classical treatment is valid in principle for a finite but unbounded system, *i.e.*, a *strictly* closed two-dimensional surface (the charged particle moving on the surface of a sphere). It may, however, be physically realized to an approximation. 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 quantum mechanically*, making the system essentially a two-dimensional classical gas of charged particles moving on the surface of the sphere. Thus, quantum mechanics helps us realize a dimensional reduction —an essentially two-dimensional closed surface.) We could then consider a finite volume fraction of an inert medium (paraffin say) occupied by the above microspheres. This system should have a measurable diamagnetic response that will be essentially classical. 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 it will be much more interesting to try out topologies other than that of a sphere and look for qualitative differences [15]. The numerically estimated value of the diamagnetic moment for a charged particle (say, electron) moving on a sphere of radius $a = 100\,\mu$m for $B \simeq 5\,$kG, $\gamma \sim 10^9\,\text{s}^{-1}$ turns out to be ~ 1 Bohr magneton per electron which is quite large. Thus, we may 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 realizable parameter values. But, the point of principle at issue would have been made. It is our hope that experimentalists may take note of this possibility.

To conclude, we have shown that a classical system of charged particles moving on a finite but *unbounded* surface (of a sphere), as described by Langevin dynamics, has a non-zero orbital diamagnetic moment. This moment can be large.

[1]This can be readily verified by making the well-known shift of the canonical momentum variable in the partition function. This also works for the case of a particle moving on the surface of a sphere.

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