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Comment

## Comment on “Classical Langevin dynamics of a charged particle moving on a sphere and diamagnetism: A surprise” by Kumar N. and Kumar K. Vijay

AVINASH A. DESHPANDE<sup>1(a)</sup>, K. VIJAY KUMAR<sup>2,3(b)</sup> and N. KUMAR<sup>1(c)</sup>

<sup>1</sup> Raman Research Institute - Bangalore, 560080 India

<sup>2</sup> CCMT, Department of Physics, Indian Institute of Science - Bangalore, 560012 India

<sup>3</sup> Department of Mechanical Engineering and Materials Science, and Department of Physics, Yale University New Haven, CT 06511, USA

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A recent numerical simulation by Kumar and Kumar [1] of the classical Langevin dynamics of a charged particle moving on a sphere placed in a uniform static magnetic field had given a non-zero orbital diamagnetic moment in the long-time limit, *i.e.*, in the steady state. This numerical result appeared as a surprise in view of the well-known Bohr-van Leeuwen (BvL) theorem on the absence of classical orbital (dia)magnetism in thermal equilibrium [2]. It has, however, been questioned [3,4] inasmuch as the Fokker-Planck (F-P) equation [4], associated with the Langevin equation [5], was pointed out to be satisfied exactly and uniquely in the steady state by the normally expected canonical probability distribution (*i.e.*, the Maxwellian velocity distribution) that does not involve the applied magnetic field, and, therefore, gives zero magnetic moment. (And this despite the fact that the F-P equation itself did explicitly contain the magnetic field as a parameter!) In the present Comment, we have specifically repeated the simulation [1] for progressively smaller values of the chosen elementary time-step  $\Delta\tau$  approaching zero, at which the magnetic moment was indeed found to extrapolate to zero. As will be discussed below, this resolves the stated disagreement. This, however, suggests an interesting possibility for realizing a finite steady-state orbital magnetic moment in certain classical systems driven by stochastic-dissipative processes which are non-Markovian, and do not obey the fluctuation-dissipation (FD) relation [6], but do lead to a steady state.

For the sake of clarity of presentation, we reproduce below the two basic Langevin equations (eqs. (3) and (4) of [1]) describing the charged-particle motion on a sphere of radius  $a$  placed in a magnetic field  $B$ . In obvious notation [1], we have

$$\ddot{\theta} - \sin\theta \cos\theta \dot{\phi}^2 = -\frac{\omega_c}{\gamma} \sin\theta \cos\theta \dot{\phi} - \dot{\theta} + \sqrt{\eta} f_\theta, \quad (1)$$

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

with the delta-correlated driving Gaussian noise,  $\langle f_\alpha(t) f_\beta(t') \rangle = \delta_{\alpha\beta} \delta(t-t')$  of zero mean and unit variance, and the overhead dots denoting differentiation with respect to the dimensionless time  $\tau = \gamma t$ . Here  $\omega_c = eB/mc$  is the cyclotron frequency,  $\gamma$  is the friction constant, while  $\eta$  parametrizes the strength of the Gaussian random noise in accordance with the FD relation [6]. These Langevin equations are known to lead to statistical equilibrium as a unique steady state in the limit  $t \rightarrow \infty$ . We are, of course, interested in the steady-state orbital magnetic moment  $\mu = -e\gamma/2c \langle \langle \mathbf{r} \times \dot{\mathbf{r}} \rangle \rangle$ . Here the double angular bracket denotes averaging over noise realizations (ensemble averaging) as well as over time.

Now, the numerical simulation [1] of the above Langevin equations, as indeed of any such stochastic equation, necessarily involves discretization of the continuous time ( $\tau$ ) parameter with an elementary discrete time step ( $\Delta\tau$ ). Here the random noises  $f_\alpha(t)$ , acting over these elementary time intervals of duration  $\Delta\tau$ , are drawn as identically independently distributed Gaussian random variables, with zero mean and a standard deviation  $\sigma$  proportional to  $\sqrt{\Delta\tau}$ , *i.e.*, as appropriate to the numerical

(a) E-mail: desh@rri.res.in

(b) E-mail: krishnamurthy.vijaykumar@gmail.com

(c) E-mail: nkumar@rri.res.in

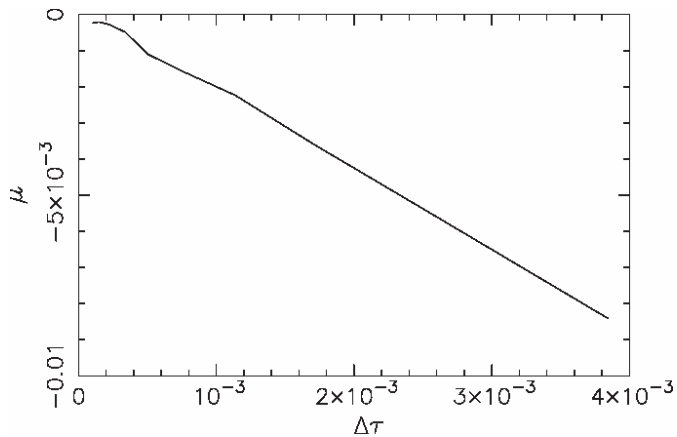


Fig. 1: Plot of ensemble-averaged steady-state orbital diamagnetic moment  $\mu$  in units of  $e\gamma a^2/2c$ , against the time step  $\Delta\tau$  used, with  $\omega_c/\gamma$  as in [1]. Note that the moment extrapolates to zero as  $\Delta\tau$  tends to zero —the Wiener limit.

simulation of a discretized Wiener process, to be discussed later following eq. (3).

In fig. 1, we have plotted the computed steady-state orbital magnetic moment  $\mu$  from this extended numerical simulation of the discretized stochastic process as a function of the elementary time step  $\Delta\tau$  chosen, keeping the other parameters such as the magnetic field and the friction coefficient fixed as in [1]. We can clearly see now that the magnitude of the steady-state diamagnetic moment  $\mu$  decreases monotonically with decreasing elementary time step  $\Delta\tau$ . Indeed, as  $\Delta\tau \rightarrow 0$ , the computed orbital moment  $\mu$  does extrapolate to zero. The  $\Delta\tau \rightarrow 0$  limit, of course, corresponds to the ideal Langevin dynamics with Gaussian white noise (a Wiener process). In this ideal limit the above stochastic dissipative process indeed leads to the standard Fokker-Planck equation [4,5,7]. This then makes the result of the earlier numerical simulation [1], as now extended to the limit  $\Delta\tau=0$ , consistent with the F-P steady-state result obtained analytically in [4], giving a zero orbital magnetic moment in the steady state —now become the thermal equilibrium!

The ideal white-noise process is, however, physically valid, strictly speaking, only for the Brownian motion of a particle having high inertia and large size relative to the fluid molecules, *e.g.*, for a silica microsphere or a colloidal particle suspended in a dense fluid [8], so that the Brownian particle of interest hardly moves on the time scale of the random molecular fluctuations on it. In the case of a light particle (*e.g.*, the electron), however, the randomly fluctuating force (thermal noise) term is expected to have a finite correlation time scale which becomes dynamically relevant now. We believe that the non-zero orbital magnetic moment obtained in the simulation [1] for a non-zero  $\Delta\tau$  arises because the latter essentially mimics such a stochastic dissipative process, namely a non-Markovian process that does, however, lead to a steady state because of the friction.

The above vanishing of the steady-state orbital magnetism in the limit  $\Delta\tau=0$  (*i.e.*, the Gaussian white

noise, or the Wiener limit), may be understood as follows. The Wiener process is described in general by a stochastic differential equation [7], which on discretization (as relevant to our numerical simulation), is of the form

$$r_i(t + \Delta t) = r_i(t) + F_i[\mathbf{r}(t)]\Delta t + \eta\sqrt{\Delta t}d\omega(t) \quad (3)$$

with  $d\omega(t)$  a normalized Gaussian noise of mean zero and variance unity. Now, in the Wiener limit ( $\Delta t \rightarrow 0$ ), we have  $\sqrt{\Delta t}/\Delta t \rightarrow \infty$  *i.e.*, the noise term infinitely dominates over the systematic force term. This is expected to totally randomize *directionally* the velocity vector  $\dot{\mathbf{r}}$ , occurring in the expression for the orbital magnetic moment  $-e\gamma/2c(\mathbf{r} \times \dot{\mathbf{r}})$ , almost instantaneously, *i.e.*, before the position vector, being the time integral of the velocity vector, has had time enough to change appreciably at all. Therefore, the vector product  $\mathbf{r} \times \dot{\mathbf{r}}$  averages to zero in the Wiener limit, as a result of complete disruption of the orbital cyclotron motion.

In contrast to this, for a non-Markovian random noise (not obeying the FD relation), the time interval  $\Delta\tau$  is necessarily finite during which the Lorentz-force-induced systematic part of the orbital motion can survive. The question of the sign as well as the magnitude of the orbital magnetic moment, however, calls for further study —of the effect of the various time scales in the problem, such as the cyclotron period, the correlation time of the non-white (colored) noise, and the related frictional relaxation, for the classical stochastic dissipative process.

In conclusion, we would like to emphasize that the simulation [1] giving a steady-state non-zero diamagnetic moment turns out to correspond essentially to a stochastically driven dissipative process which is Gaussian but not Markovian —indeed not obeying the FD relation [6,9] for a constant friction coefficient  $\gamma$ . Thus, we have here a steady state rather than a state of thermal equilibrium. When extended to the Wiener limit  $\Delta\tau \rightarrow 0$ , however, the steady state does indeed become a state of thermal equilibrium, and the moment vanishes in agreement with [4].

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