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A Langevin Approach to a Classical Brownian Oscillator in an Electromagnetic Field

J. S. Espinoza Ortiz¹, F. C. Bauke², R. E. Lagos³

¹Departamento de Física, IFQC, Universidade Federal de Goiás, Catalão, Goiás 75704/020, Brasil.

²Instituto de Física *Gleb Wataghin*, UNICAMP, Campinas, São Paulo 13083/970, Brasil.

³Departamento de Física, IGCE, UNESP, Rio Claro, São Paulo 13500/970, Brasil.

E-mail: jsespino@physics.org

Abstract. We consider a charged Brownian particle bounded by an harmonic potential, embedded in a Markovian heat bath and driven from equilibrium by external electric and magnetic fields. We develop a quaternionic-like (or Pauli spinor-like) representation, hitherto exploited in classical Lorentz related dynamics. Within this formalism, in a very straight forward and elegant fashion, we compute the exact solution for the resulting generalized Langevin equation, for the case of a constant magnetic field. For the case the source electromagnetic fields satisfy Maxwell's equations, yielding spinor-like Mathieu equations, we compute the solutions within the JWKB approximation. With the solutions at hand we further compute spatial, velocities and crossed time correlations. In particular we study the (kinetically defined) nonequilibrium temperature. Therefore, we can display the system's time evolution towards equilibrium or towards non equilibrium (steady or not) states.

1. Introduction

The ubiquitous Brownian motion remains an outstanding paradigm in modern physics [1, 2, 3, 4, 5, 6, 7, 8] (and references therein). The theoretical framework consisting of Kramers equation (a Fokker-Planck equation in phase space), Smoluchowski equation (asymptotic or overdamped contraction of the latter) and the associated stochastic Langevin equation, have been widely applied to diverse problems, such as: Brownian motion in potential wells, chemical reactions rate theory, nuclear dynamics, stochastic resonance, surface diffusion, general stochastic processes and evolution of nonequilibrium systems, in both classical and quantum contexts. More recent applications include thermodynamics of small systems, molecular motors, chemical and biological nanostructures in the burgeoning field of nanotechnology, mesoscopic motors power output and efficiency. It took approximately sixty years to report exact solutions for the Brownian motion of a charged particle in uniform and static electric and/or magnetic fields [6, 7, 8, 9]. Here we outline the extension of our previous work [5, 6, 7, 8] and consider a charged Brownian oscillator under electromagnetic fields.

In section 2 we write down the Langevin equation for a charged particle under an harmonic potential and external electric and magnetic fields (as reported in [6, 7] homogeneous forces can be included straightforwardly into our formalism). In section 3 we compute the exact solution of Langevin's equation when considering a time independent magnetic field, via a novel method (spinors and Pauli matrices), compute spatial, velocities and crossed time correlations; and outline some applications of our result, in particular we study the (kinetically defined)



non equilibrium temperature. In section 4 we present the approximate (JWKB) solution of Langevin's equation under an electromagnetic field satisfying Maxwell equations. Finally in section 5 we present further applications and extensions of our work.

2. Langevin Equation for a Charged Brownian Oscillator under Electromagnetic Fields

Lets us consider a charged (carrier) Brownian oscillating particle, in contact with a reservoir at temperature T_R , under the influence of electromagnetic fields. The Langevin equation [5, 6, 7, 8, 9, 10, 11] is given by

$$m \frac{d^2 \mathbf{x}}{dt^2} = -m\lambda \frac{d\mathbf{x}}{dt} - m\omega_0^2 \mathbf{x} + q \left(\mathbf{E} + \frac{1}{c} \frac{d\mathbf{x}}{dt} \times \mathbf{B} \right) + \mathbf{F}^r(t) \quad (1)$$

where $\mathbf{x}$ is the carrier's position (the carrier's velocity is $\mathbf{v} = d\mathbf{x}/dt$), m the mass, q the charge, $m\lambda$ Stokes' force constant ($\lambda^{-1} = \tau_c$, collision time), ω_0 Hooke's frequency, c light velocity (in CGS units) and $\mathbf{E}$ & $\mathbf{B}$ the Electric and Magnetic external fields, respectively. $\mathbf{F}^r(t)$ is the random Brownian force, white Markovian noise with statistics (mean and correlations) given by [6, 7, 8, 9, 10, 11]

$$\langle \mathbf{F}^r(t) \rangle = \mathbf{0} \quad , \quad \langle F_i^r(t) F_j^r(t') \rangle = 2\Gamma \delta_{ij} \delta(t - t') \quad (2)$$

where the noise strength is given by $\Gamma = m\lambda k_B T_R$ (Fluctuation Dissipation Theorem [1, 2, 3]).

We consider homogeneous fields (constant or solely time dependent), choose $\mathbf{B} = B\hat{\mathbf{z}}$ and with the convenient definitions $\mathbf{f} = q\mathbf{E}/m$, $\mathbf{f}^r = \mathbf{F}^r/m$ and cyclotron frequency $\omega_c = qB/mc$, the Brownian Lorentz Langevin oscillator equations are cast as

$$\begin{aligned} \ddot{x} &= -\lambda \dot{x} + \omega_c \dot{y} - \omega_0^2 x + f_x + f_x^r, \\ \ddot{y} &= -\lambda \dot{y} - \omega_c \dot{x} - \omega_0^2 y + f_y + f_y^r, \\ \ddot{z} &= -\lambda \dot{z} - \omega_0^2 z + f_z + f_z^r. \end{aligned} \quad (3)$$

Since the z (non magnetic) component is uncoupled from the xy (magnetic) motion hereafter we ignore the former, and when needed we call in the exact solution [1, 2, 3].

Define sigma real matrices (2×2), a commutative quaternion subalgebra. A is a “ σ -matrix” if the real matrix A can be cast as

$$A = \begin{pmatrix} a_1 & -a_2 \\ a_2 & a_1 \end{pmatrix} = a_1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + a_2 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = a_1 + a_2 \sigma, \quad \sigma^2 = -1.$$

As in quaternions we define the conjugate $\tilde{A}$, the norm $\|A\|$ and the argument $\arg(A)$ associated to $A = a_1 + a_2 \sigma$, respectively by $\tilde{A} = a_1 - a_2 \sigma$, $\|A\|^2 = A\tilde{A} = \det A = a_1^2 + a_2^2$, $\arg(A) = a_2/a_1$. It follows $A^{-1} = \tilde{A}/\|A\|^2$. Furthermore since $\sigma = i\sigma_y$ (the y component of Pauli's σ matrix) [10] we obtain the (de Moivre like) relations

$$\exp(A) = \exp(a_1) (\cos a_2 + \sigma \sin a_2) \quad , \quad \exp(iA) = \exp(ia_1) (\cosh a_2 + i\sigma \sinh a_2) \quad ,$$

and from the last equations, straightforward expressions for several functions such as $\cos A$, $\sin A$, $\ln A$, A^p , are obtained. In particular: $\cos A = \cos a_1 \cosh a_2 - \sigma \sin a_1 \sinh a_2$, $\sin A = \sin a_1 \cosh a_2 + \sigma \cos a_1 \sinh a_2$, $\ln A = \|A\| + \sigma \arctan \arg A$, and

$$\sqrt{A} = \sqrt{\frac{\|A\| + a_1}{2}} + \text{sgn}(a_2) \sigma \sqrt{\frac{\|A\| - a_1}{2}} \quad (4)$$

for $a_1 > 0$ (for $a_1 < 0$, we choose the convention $\sqrt{A} = i\sqrt{-A}$).

Now, define the “spinors”

$$q = \begin{pmatrix} x \\ y \end{pmatrix}, \quad \phi = \begin{pmatrix} f_x + f_x^r \\ f_y + f_y^r \end{pmatrix} = f + f^r \quad (5)$$

and as usual, the adjoint spinor $q^\dagger = (x, y)$. With $\Lambda_c = \lambda + \omega_c \sigma$, equation (3) is cast in the form

$$\frac{d^2 q}{dt^2} + \Lambda_c \frac{dq}{dt} + \omega_0^2 q = \phi. \quad (6)$$

Now, we proceed to solve this system of two second order linear inhomogeneous coupled equations, for two cases, namely: constant magnetic field (section 3) and plane waves fields, solutions of Maxwell equations (section 4).

3. Exact Solution for constant Magnetic Field

For a constant magnetic field, equation (6) has an exact solution, and was derived in a related, more general context [11, 12]. Here we apply a novel method of solution hinging on the quaternion scheme presented in the previous section. We believe this method to be more straightforward since in the quaternion commutative sub algebra, our resulting equations can be considered as representing a bona fide one dimensional problem. At the very end of the calculations, yielding observable quantities, only then we explicitly decompose any σ -matrices (say A) into its scalar components $A = a_1 + a_2 \sigma$.

Disregarding the homogeneous solution (transient), the exact solution of equation (6) for constant magnetic field, is given by [13],

$$q(t) = \int_0^t d\tau G(t - \tau) (f(\tau) + f^r(\tau)) \quad (7)$$

with the Green function

$$G(t) = \frac{1}{\Omega_c} \sin(\Omega_c t) \exp\left(-\frac{1}{2}\Lambda_c t\right) = g_1(t) + \sigma g_2(t) \quad (8)$$

where $\Omega_c = \sqrt{\omega_0^2 - \Lambda_c^2/4}$. We can readily compute the (spinor) velocity $v(t) = dq(t)/dt$. Now, with a minimum of algebra we can compute all quadratic correlations $C_{ab}(t, \tau) = \langle a(t)b(\tau) \rangle$ with the rules given by equation (2), where a and b are any combination of the spinor components of position $q(t)$ and velocity $v(t)$. The $z(t)$ and $v_z(t)$ components are easily computed from either spinor component by just setting $\omega_c = 0$. All expressions are readily integrated into elementary functions. In particular the case of time independent electric field hereafter considered in this section. Some interesting correlations are

$$K(t) = \frac{1}{2} m \langle v^\dagger(t) v(t) + v_z^2(t) \rangle = \frac{3}{2} k_B T(t), \quad (9)$$

$$V(t) = \frac{1}{2} m \omega_0^2 \langle q^\dagger(t) q(t) + z^2(t) \rangle, \quad (10)$$

yielding a kinetic time dependent definition of temperature [6, 7, 8] and average potential energy, respectively. For zero external fields both equal time correlations asymptotically converge towards the classical equipartition theorem value $3k_B T_R/2$. Interesting preliminary results involve the transition from a normal carrier profile to a hot carrier profile [8] as a mode softening process occurs ($\omega_0 \rightarrow 0$).

4. Approximate (JWKB) solution for a Maxwell Electromagnetic Field

When the external electromagnetic fields are not constant some approximations are necessary in order to produce tractable and relevant results (for example in sun activated photovoltaic devices [14]). In particular for electromagnetic plane monochromatic (ω) waves propagating in the $\hat{x}$ direction and satisfying Maxwell equations [15], we have $\mathbf{B} = \hat{z}B \cos \omega t$ and $\mathbf{E} = \hat{y}B \cos \omega t$. After taking real parts (as usual in classical physics), the Brownian Maxwell Langevin equation is cast as:

$$\frac{d^2q}{dt^2} + \Lambda(t)\frac{dq}{dt} + \omega_0^2 q = f + f^x, \quad (11)$$

again, as before, we decouple the planar xy motion from the perpendicular z motion. In this case we have $f_x = 0$ and $f_y = c\omega_c \cos \omega t$, and $\Lambda(t) = \lambda + \sigma\omega_c \cos \omega t$. Due to the time dependent $\Lambda(t)$ dissipative factor, the exact solution involves spinorial Mathieu functions. Nevertheless we can write the JWKB solutions [16], certainly a good approximation for small field $w_c \ll \lambda$,

$$q(t) = \int_0^t d\tau G(t, \tau) (f(\tau) + f^x(\tau)), \quad (12)$$

$$G(t, \tau) = \frac{1}{\sqrt{\Omega(t)\Omega(\tau)}} \sin \left(\int_\tau^t d\theta \Omega(\theta) \right) \exp \left(-\frac{1}{2} \int_\tau^t d\theta \Lambda(\theta) \right), \quad (13)$$

where $\Omega(t) = \sqrt{\omega_0^2 - \Lambda^2(t)/4}$. Notice, in this case that the Green function given in equation (11) is not dependent in the time difference $t - \tau$ as in the exact solution in section 3 for the constant magnetic field case, and stands as the JWKB approximation for damped spinor Mathieu functions. Correlation functions in this case cannot be reduced to elementary functions as in the previous case.

5. Conclusions and Future work

In this short communication, we outlined and presented a novel method to compute solutions for the Langevin equation for a charged Brownian oscillator under external fields, in particular electromagnetic fields. Two cases were considered, namely: for the constant magnetic field, the exact solution was presented; and for both time dependent electric and magnetic fields satisfying Maxwell equations, the approximate JWKB solution was obtained. We outlined too, how to compute quadratic (two time) correlation functions, related to relevant physical quantities such as nonequilibrium temperature. These correlation functions will allow us to study the evolution of this nonequilibrium Brownian process, the oscillator's dynamics and as mentioned above the mode softening transition. For the case of constant magnetic field work is in progress, and results will be presented in a subsequent long paper. As for the JWKB solution, work is at the preliminary stage. This work is relevant in different fields besides physics, including biology and economics. It contributes to further understand small (nano) systems, may they be mechanical, chemical or biological.

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