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Theory of Brownian motion of a massive particle in spaces with curvature and torsion

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Abstract. With the motivation of studying the diffusive propagation of massive particles in crystals with defects, we develop a theory of Brownian motion of a massive particle, including the effects of inertia, in spaces with curvature and torsion. This is done with the help of a recently discovered *nonholonomic mapping principle*, which carries known classical equations of motion in Euclidean space into non-Euclidean space. In particular, the known Langevin equation in Euclidean space goes over into a Langevin equation in spaces with curvature and torsion from which we derive, in this note, the Kubo and Fokker–Planck equations satisfied by the particle distribution as a function of time in such spaces. The possible relevance of these equations to particle propagation in crystals with defects is discussed.

Since defects in crystals can be described geometrically by a nonvanishing curvature and torsion [1, 2], there is a definite need to find the correct Fokker–Planck equation for the distribution of particles moving through such spaces. In flat space, the classical equation of a massive point particle in a thermal environment reads

$$m\ddot{x}_t^i = f_t^i + \bar{f}_t^i \tag{1}$$

where f_t^i is an arbitrary time-dependent external force and $\bar{f}_t^i$ is a stochastic force caused by the thermal fluctuations (we use subscripts for the time variable). The stochastic force may be modelled by a bath of harmonic oscillators of all frequencies ω as

$$\bar{f}_t^i = \int_0^\infty \mathrm{d}\omega\, \lambda_\omega \dot{X}_{\omega t}^i. \tag{2}$$

The oscillator coordinates satisfy the equations of motion

$$\ddot{X}_{\omega t}^i + \omega^2 X_{\omega t}^i = \lambda_\omega \dot{x}_t^i \tag{3}$$

the right-hand side arising from the back-reaction of the particle.

Solving (3) with respect to $X_{\omega t}^i$ we find (2) as a functional of $\dot{x}^i$. Assuming an equal coupling $\lambda_\omega \equiv \sqrt{2\gamma/\pi}$ for all oscillators, we obtain the stochastic differential equation

$$m\ddot{x}_t^i + \gamma\dot{x}_t^i - f_t^i = \eta_t^i \tag{4}$$

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where η_t^i is called the *noise variable*. It has the Fourier decomposition

$$\eta_t^i = (2\gamma/\pi)^{1/2} \int_0^\infty \mathrm{d}\omega\, [\dot{X}_\omega^i \cos\omega t - X_\omega^i \sin\omega t]. \tag{5}$$

For any given phase-space distribution $\rho^B = \rho^B(\dot{X}, X)$ of $\dot{X}_\omega^i$ and X_ω^i, equation (4) becomes a classical Langevin equation with noise averages being defined as mean values with respect to the distribution ρ^B. In thermal equilibrium, ρ^B follows the Boltzmann law $\sim \exp(-H^B/kT)$, where the bath Hamiltonian is a sum of the oscillator Hamiltonians: $H^B = \int \mathrm{d}\omega\, (\dot{X}_\omega^2 + \omega^2 X_\omega^2)/2$. The associated noise i is Gaussian, and completely specified by its vanishing expectation and its two-point correlation function:

$$\langle \eta_t^i \rangle = 0 \qquad \langle \eta_t^i \eta_{t'}^j \rangle = 6\gamma k T \delta^{ij} \delta(t - t'). \tag{6}$$

According to the nonholonomic mapping principle proposed in [3, 4], the infinitesimal coordinate transformation $\mathrm{d}x^i = e^i{}_\mu(q)\mathrm{d}q^\mu$ carries classical Euclidean equations of motion correctly into spaces with curvature and torsion [5]. The geometry in this space is defined by the metric $g_{\mu\nu} = e^i{}_\mu e^i{}_\nu$ and the affine connection $\Gamma_{\mu\nu}{}^\lambda = e_i{}^\lambda \partial_\mu e^i{}_\nu$. The torsion resides in the antisymmetric part of the affine connection, $S_{\mu\nu}{}^\lambda = (\Gamma_{\mu\nu}{}^\lambda - \Gamma_{\nu\mu}{}^\lambda)/2$, and is a tensor [6]. Curvature is signalled by noncommuting derivatives of the nonholonomic quantities $e^i{}_\lambda$, the curvature tensor being given by $R_{\mu\nu\lambda}{}^\kappa = e_i{}^\kappa(\partial_\mu\partial_\nu - \partial_\mu\partial_\nu)e^i{}_\lambda$. Thus, in a curved space, $e_i{}^\mu(q_t)$ are no proper functions, failing to satisfy Schwarz' criterion.

Since the Langevin equation (4) is a classical equation of motion, its image under the nonholonomic mapping $\mathrm{d}x^i = e^i{}_\mu(q)\mathrm{d}q^\mu$ should be the correct Langevin equation in spaces with curvature and torsion. The result is

$$m(\ddot{q}_t^\mu + \Gamma_{\sigma\nu}{}^\mu \dot{q}_t^\sigma \dot{q}_t^\nu) + \gamma \dot{q}_t^\mu - f_t^\mu = e_i{}^\mu(q_t)\eta_t^i. \tag{7}$$

To obtain physical consequences we must find equations in which the nonholonomic quantities $e_i{}^\mu(q_t)$ are eliminated in favour of the well-defined geometrical quantities $g_{\mu\nu}(q)$ and $\Gamma_{\mu\nu}{}^\lambda(q)$. This is possible by deriving from (7) Kubo's stochastic Liouville equation and the Fokker–Planck equation with inertia.

For this we rewrite the Langevin equation as a system of two first-order differential equations

$$\dot{q}_t^\mu = \frac{1}{m} g^{\mu\nu}(q_t) p_\nu^t \tag{8}$$

$$\begin{aligned}\dot{p}_\mu^t &= -\frac{1}{m}(\Gamma^{\sigma\nu}{}_\mu - g^{\sigma\lambda} g^{\nu\alpha} \partial_\lambda g_{\mu\alpha}) p_\sigma^t p_\nu^t - \frac{\gamma}{m} p_\mu^t + f_t^\mu + e_i^\mu \eta_t^i \\ &\equiv -F_\mu^t + e_\mu^i \eta_t^i \end{aligned}\tag{9}$$

the last equation defining a total apparent force F_μ^t. This force is not obviously a vector under general coordinate transformations, due to the presence of the connection. However, the covariance of the Langevin equation (7) ensures the covariance of equation (9).

At each time t, the system following equations (8) and (9) is in a microscopic state with the distribution function $\delta(p - p_t)\delta(q - q_t)$. This can be thought of as a conditional distribution function determining the distribution of p_μ and q^μ for a given initial distribution function $\delta(p - p^0)\delta(q - q_0)$. If the initial values of p_μ^t and q_t^μ are distributed with the probability density $\rho = \rho(p^0, q_0)$, the distribution function at any later time t can be found by an average over the initial distribution

$$\rho_t^\eta(p, q) = \int \mathrm{d}p^0\, \mathrm{d}q_0\, \rho(p^0, q_0)\delta(p - p^t)\delta(q - q_t) \tag{10}$$

where $q_t^\mu = q_t^\mu(p^0, q_0)$ and $p_\mu^t = p_\mu^t(p^0, q_0)$ are solutions of the system (8), (9) with the initial conditions $p_\mu^{t=0} = p_\mu^0$ and $q_{t=0}^\mu = q_0^\mu$. By taking a time derivative of (10) and making use of both (8) and (9), we find Kubo's stochastic Liouville equation

$$\partial_t \rho_t^\eta = \hat{L}(\eta_t)\rho_t^\eta \tag{11}$$

with $\hat{L}(\eta_t)$ being the noise-dependent Liouville operator

$$\hat{L}(\eta_t) = -\frac{\partial}{\partial q^\mu} \circ g^{\mu\nu}\frac{p_\nu}{m} + \frac{\partial}{\partial p_\mu} \circ [F_\mu(p,q) - e_\mu^i \eta_t^i] \tag{12}$$

where the symbol $\circ$ stands for composition of operators. It is straightforward to verify the invariance of the Liouville operator and, hence, of Kubo's equation with respect to general coordinate transformations.

A solution of Kubo's stochastic equation (11) is a noise-dependent distribution function which determines the probability of finding a particle in an infinitesimal volume dq by

$$\mathrm{d}P_t(q) = \mathrm{d}q \int \mathrm{d}p\, \langle \rho_t^\eta(p,q)\rangle \equiv \mathrm{d}q \int \mathrm{d}p\, \rho_t(p,q). \tag{13}$$

It follows then from (10) that $\int \mathrm{d}P_t\,(q) = \int \mathrm{d}P_0\,(q) = 1$, i.e. the temporal evolution of the probability distribution described by Kubo's equation (11) is unitary.

Due to the locality of the noise correlation function in (6), it is possible to derive a Fokker–Planck equation which governs the temporal evolution of the noise-averaged distribution $\rho_t(p,q)$. For this purpose let us first calculate the average $\varphi_t^i = \langle \eta_t^i \delta(p - p^t)\delta(q - q_t)\rangle$. Generalizing the partial integration formula $\int \mathrm{e}^{-a\eta^2/2}\eta f(\eta)\,\mathrm{d}\eta = a^{-1}\int \mathrm{e}^{-a\eta^2/2} f'(\eta) = -a^{-1}\int \partial_\eta \mathrm{e}^{-a\eta^2/2} f(\eta)$ to any Gaussian noise, we find

$$\begin{aligned}\varphi_t^i &= \int_{-\infty}^{\infty} \mathrm{d}t' \langle \eta_t^i \eta_{t'}^j\rangle \left\langle \frac{\delta}{\delta\eta_{t'}^j}\delta(p - p^t)\delta(q - q_t)\right\rangle \\ &= -6\gamma kT \left\langle \left(\frac{\partial}{\partial p_\mu} \circ \frac{\delta p_\mu^t}{\delta \eta_t^i} + \frac{\partial}{\partial q^\mu} \circ \frac{\delta q_t^\mu}{\delta \eta_t^i}\right)\delta(p - p^t)\delta(q - q_t)\right\rangle \end{aligned} \tag{14}$$

where we have used the explicit form of the two-point noise correlation function (6). To calculate the variational derivatives of dynamical variables with respect to noise in (14), we formally integrate (8) and (9):

$$p_\mu^t = p_\mu^0 + \int_0^t \mathrm{d}t'\,(-F_\mu^{t'} + e_\mu^i \eta_{t'}^i) \tag{15}$$

$$q_t^\mu = q_0^\mu + \frac{1}{m}\int_0^t \mathrm{d}t'\, g^{\mu\nu}(q_{t'})p_\nu^{t'}. \tag{16}$$

Taking the variational derivative of (15) we obtain

$$\frac{\delta p_\mu^t}{\delta \eta_{t'}^i} = -\int_{t'}^t \mathrm{d}t'' \left[\frac{\delta F_\mu^{t''}}{\delta \eta_{t'}^i} - \eta_{t''}^j \frac{\delta e_\mu^j(q_{t''})}{\delta \eta_{t'}^i}\right] + \int_{t'}^t \mathrm{d}t'' e_i^\mu(q_{t''})\delta(t'' - t'). \tag{17}$$

The Langevin equation (9) is causal which implies that $p_{t''}^\mu$ or $q_{t''}^\mu$ depend on $\eta_{t'}^i$ only for $t'' > t'$. This has been used to restrict the integration range in (17). The first integral on the right-hand side of (17) tends to zero as t' approaches t, whereas the second integral is not uniquely determined at $t = t'$, since it contains a Heaviside function at zero argument. The calculation of the contribution of $\delta p_\mu^t/\delta\eta_t^i$ to (θ) requires therefore a regularization. We replace the delta-function in the correlator (6) by a smooth would-be delta-function function $\delta_\epsilon(t - t')$, of width ϵ, satisfying $\int_{-\infty}^{\infty} \mathrm{d}t\,\delta_\epsilon(t) = 1$ and $\delta_\epsilon(t) = \delta_\epsilon(-t)$. Such a regularization can be achieved by retaining a weak dependence on ω in the coupling constant λ_ω. With this regularization, we have to replace $\delta p^t_\mu/\delta\eta^i_t$ in (14) by

$$\int_{-\infty}^{\infty} \mathrm{d}t'\,\delta_\epsilon(t-t')\frac{\delta p^t_\mu}{\delta\eta^i_{t'}} = e^i_\mu(q_t)\int_{-\infty}^{\infty}\mathrm{d}t'\,\delta_\epsilon(t-t')\theta(t-t') = \tfrac{1}{2}e^i_\mu(q_t) \qquad (18)$$

where we have dropped the contribution of the first integral of (17) since it vanishes for $\epsilon \to 0$.

Considering analogously $\delta q^\mu_t/\delta\eta^i_{t'}$, we conclude that the latter variational derivative vanishes as t' approaches t. Averaging φ^i_t with respect to the initial distribution $\rho(p_0, q_0)$ we find the following relation

$$\int \mathrm{d}p_0\,\mathrm{d}q_0\,\rho(p_0,q_0)\varphi^i_t = \langle\eta^i_t\rho^\eta_t\rangle = -3\gamma kT e^i_\mu\frac{\partial}{\partial p_\mu}\rho_t. \qquad (19)$$

Taking the noise average of Kubo's stochastic equation (11) and making use of (19), we end up with the Fokker–Planck equation with inertia associated with the Langevin equation (7):

$$\partial_t\rho_t = \hat{L}_T\rho_t \qquad (20)$$

$$\hat{L}_T = -\frac{\partial}{\partial q^\mu}\circ g^{\mu\nu}\frac{p_\nu}{m} + \frac{\partial}{\partial p_\mu}\circ\left[F_\mu(p,q) + 3\gamma kT g^{\mu\nu}\frac{\partial}{\partial p_\nu}\right]. \qquad (21)$$

Thus, we have eliminated the nonholonomic mapping functions in favour of the well-defined affine connection and metric. Integrating (20) over the whole phase space we verify at the probability conservation law: $\mathrm{d}/\mathrm{d}t\int\mathrm{d}p\,\mathrm{d}q\,\rho_t = 0$, where we have used the fact of vanishing surface integrals occurring upon the integration of the right-hand side of (20).

An application of equations (20), (21) to the diffusion of particles in crystals with defects is, unfortunately, not straightforward. The motion of a particle is sensitive to the geometry of defects only if this particle measures distances by counting steps when hopping through the crystal. Electrons qualify for this only in the tight-binding approximation. In this approximation, the hopping probability which is the result of quantum tunnelling depends very strongly on the elastic distortions of the crystal. In the above geometrical description of the system, elastic distortions play the role of general coordinate transformations. The Langevin equation (7) is invariant under such transformations by construction, while the physical hopping probability is not. In order to apply the equation, such a dependence must be included, and averaged at the end over the phonon bath. An additional problem is the calculation of the classical limit within the tight-binding approximation. Initial attempts to study the Brownian motion of a particle in a crystal with defects have not addressed these issues [8].

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