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On the stochastic Lagrangian and a new derivation of the Schrödinger equation

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Abstract. We obtain an expression for the stochastic Lagrangian as used in stochastic mechanics in a straightforward manner without obtaining the singular terms of Guerra's approach. We then present a new derivation of the Schrödinger equation.

1. Introduction

In classical mechanics one usually considers the following system when discussing the motion of a particle of mass m under the influence of a scalar potential $V(\boldsymbol{q}, t)$ and a vector potential $\boldsymbol{A}(\boldsymbol{q}, t)$ in R^3 :

$$
\begin{aligned}
m\ddot{\boldsymbol{q}} &= -\nabla V - \frac{\partial \boldsymbol{A}}{\partial t} - (\nabla \wedge \boldsymbol{A}) \wedge \dot{\boldsymbol{q}} \\
L &= \frac{m}{2}\dot{\boldsymbol{q}}\cdot\dot{\boldsymbol{q}} + \boldsymbol{A}\cdot\dot{\boldsymbol{q}} - V \\
H &= \boldsymbol{p}\cdot\dot{\boldsymbol{q}} - L
\end{aligned}
$$

where $\boldsymbol{q}$ denotes the particle's position, $\dot{\boldsymbol{q}}$ denotes its velocity and $\boldsymbol{p} = m\dot{\boldsymbol{q}} + \boldsymbol{A}$ is the canonical momentum. The Lagrangian L and Hamiltonian H are calculated as above. Classical solutions of the equation of motion can be obtained by finding those $\boldsymbol{q}$ which minimise $\int L\,\mathrm{d}t$ or which ensure that

$$
\dot{H} = \frac{\partial V}{\partial t} - \frac{\partial \boldsymbol{A}}{\partial t}\cdot\dot{\boldsymbol{q}}.
$$

The canonical momentum $\boldsymbol{p}$ can also be realised as ∇S where S ($= \int L\,\mathrm{d}t$) satisfies the Hamilton–Jacobi equation

$$
-\frac{\partial S}{\partial t} = \frac{1}{2m}(\nabla S - \boldsymbol{A})\cdot(\nabla S - \boldsymbol{A}) + V.
$$

We have suppressed the fundamental constants of electric charge and the speed of light in the above by setting $e = c = 1$. We omit the more technical requirements on $\boldsymbol{q}, S$, etc as we only wish to remind the reader of the usual system studied.

In stochastic mechanics as devised by Nelson (1985) and developed by Guerra and Morato (1983) one immediately comes across a problem in the definition of a velocity or any derivative with respect to time. The central theme of stochastic mechanics is to model the position of the particle by use of a diffusion process. The paths of the process are continuous but not differentiable. Nelson developed a stochastic Newton equation while other authors developed a stochastic Lagrangian and variational principle approach. In this study we are going to use the Hamiltonian in order to model the motion of our particle. The study is structured as follows. We first develop a new derivation of the stochastic Lagrangian by addressing the question of measurement and secondly we present a new derivation of the Schrödinger equation by requiring the rate of change of energy to be the same as in classical mechanics.

2. The stochastic Lagrangian

Let our diffusion process have the Itô equation

$$\mathrm{d}\boldsymbol{q}_t = \boldsymbol{b}(\boldsymbol{q}_t, t)\mathrm{d}t + \sqrt{\nu}\,\mathrm{d}\boldsymbol{B}_t$$

where $\nu > 0$ is the diffusion constant and $\boldsymbol{B}_t$ is a Brownian motion on R^3. Let F_t be the usual filtration generated by the sets $\{\boldsymbol{B}_u : u \leq s\}$ for $s \leq t$. For suitable functions $f(\boldsymbol{q}, t)$ we have the Itô equation

$$\mathrm{d}f(\boldsymbol{q}_t, t) = \left(\frac{\partial f}{\partial t} + \boldsymbol{b}\cdot\nabla f + \frac{\nu}{2}\Delta f\right)\mathrm{d}t + \sqrt{\nu}\nabla f\cdot\mathrm{d}\boldsymbol{B}_t.$$

The reader might consult Øksendal (1985) for a good introduction to stochastic processes and stochastic differential equations. In order to derive a stochastic Lagrangian we have to be able to accommodate the classical quantities $\dot{\boldsymbol{q}}$, $\dot{\boldsymbol{q}}\cdot\boldsymbol{A}$ and $\dot{\boldsymbol{q}}\cdot\dot{\boldsymbol{q}}$. To calculate the stochastic analogues of these quantities we use the simple ideas of measurement and averaging. Classically we have

$$\begin{aligned}
\dot{\boldsymbol{q}}(r) &= \lim_{t\to r}(\boldsymbol{q}(t) - \boldsymbol{q}(r))/(t-r)\\
\dot{\boldsymbol{q}}(r)\cdot\boldsymbol{A}(\boldsymbol{q}(r), r) &= \lim_{t\to r}(\boldsymbol{q}(t) - \boldsymbol{q}(r))\cdot\boldsymbol{A}(\boldsymbol{q}(r), r)/(t-r)\\
\dot{\boldsymbol{q}}(r)\cdot\dot{\boldsymbol{q}}(r) &= \lim_{t\to s\to r}(\boldsymbol{q}(t) - \boldsymbol{q}(s))\cdot(\boldsymbol{q}(s) - \boldsymbol{q}(r))/(t-s)(s-r).
\end{aligned}$$

The last of these expressions is the crucial one in what follows. We have to take expectations of our measured quantities with respect to the filtration F_r in order to obtain well defined expressions. We proceed as below. The velocity is represented by

$$\lim_{t\to r} E[\boldsymbol{q}_t - \boldsymbol{q}_r | F_r]/(t-r)$$

and a quick use of Itô's equation for $\boldsymbol{q}_t$ shows that this is merely $\boldsymbol{b}(\boldsymbol{q}_r, r)$. When one considers $\boldsymbol{A}\cdot\dot{\boldsymbol{q}}$ one has a choice to make. Does one consider

$$\lim_{t\to r} E[(\boldsymbol{q}_t - \boldsymbol{q}_r)\cdot\boldsymbol{A}(\boldsymbol{q}_r, r)|F_r]/(t-r)$$

or

$$\lim_{t\to r} E[\boldsymbol{A}(\boldsymbol{q}_t, t)\cdot(\boldsymbol{q}_t - \boldsymbol{q}_r)|F_r]/(t-r)?$$

These two expressions are markedly different, the first being equal to

$$\boldsymbol{b}(\boldsymbol{q}_r, r)\cdot\boldsymbol{A}(\boldsymbol{q}_r, r)$$

whilst the second is equal to

$$\boldsymbol{b}(\boldsymbol{q}_r, r)\cdot\boldsymbol{A}(\boldsymbol{q}_r, r)+\nu\nabla\cdot\boldsymbol{A}(\boldsymbol{q}_r, r).$$

We simply take the average of these two expressions to obtain

$$\boldsymbol{b}\cdot\boldsymbol{A}+\frac{\nu}{2}\nabla\cdot\boldsymbol{A}.$$

The divergence term has arisen because of the nature of the Itô equation and is most often referred to as the Itô correction. The analogue for the third of our expressions can now be written down as we have done all the work required in the previous calculation. We replace $\dot{\boldsymbol{q}}\cdot\dot{\boldsymbol{q}}$ by

$$\boldsymbol{b}\cdot\boldsymbol{b}+\nu\nabla\cdot\boldsymbol{b}$$

the coefficient of the divergence being ν not $\nu/2$ since we have no choice in our order of measurement. The important feature of this analogous term for $\dot{\boldsymbol{q}}\cdot\dot{\boldsymbol{q}}$ is that is a nice geometric object and is well defined. If one refers to Nelson (1985) and follows his account of Guerra's derivation of his analogue for $\dot{\boldsymbol{q}}\cdot\dot{\boldsymbol{q}}$ one observes that there is a singular term present, namely one of order $(\mathrm{d}t)^{-1}$. This term is ignored in the application of their variational principle. We must also point out that Guerra derives his expressions for motion in a manifold. Our methods may be applied to this most general problem in a similar way to that used herein (Davies 1989) and it is of interest to note that we do not obtain any curvature terms in the derivation of the stochastic Lagrangian.

The general principle to be gleaned from the above is that one has correction terms dependent on the diffusion constant arising from classical quantities involving $\dot{\boldsymbol{q}}$. Finally we write our stochastic Lagrangian as

$$L=\frac{m}{2}(\boldsymbol{b}\cdot\boldsymbol{b}+\nu\nabla\cdot\boldsymbol{b})+\boldsymbol{A}\cdot\boldsymbol{b}+\frac{\nu}{2}\nabla\cdot\boldsymbol{A}-V$$

which is equivalent to that used by previous authors. We emphasise that we have not made use of conditioning into the future or of backward drifts.

3. The Schrödinger equation

Having obtained the stochastic Lagrangian, the corresponding stochastic Hamiltonian can be written as

$$\begin{aligned}H&=\boldsymbol{p}\cdot\boldsymbol{b}+\frac{\nu}{2}\nabla\cdot\boldsymbol{p}-L\\&=\boldsymbol{p}\cdot\boldsymbol{b}+\frac{\nu}{2}\nabla\cdot\boldsymbol{p}-\frac{m}{2}(\boldsymbol{b}\cdot\boldsymbol{b}+\nu\nabla\cdot\boldsymbol{b})-\boldsymbol{A}\cdot\boldsymbol{b}-\frac{\nu}{2}\nabla\cdot\boldsymbol{A}+V\end{aligned}$$

where $\boldsymbol{p}$ is some function of $\boldsymbol{q}_t$ and t as yet to be determined. Let the diffusion process have a density $\rho = \exp(2R)$ where R is some real-valued scalar function of position and time. The density satisfies the differential equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(\frac{\nu}{2}\nabla\rho - \boldsymbol{b}\rho\right)$$

and setting $\boldsymbol{b} = \nu\nabla R + \boldsymbol{v}$ reduces this to the simpler form

$$-\frac{\partial R}{\partial t} = \boldsymbol{v}\cdot\nabla R + \frac{1}{2}\nabla\cdot\boldsymbol{v}.$$

We require that

$$\frac{\mathrm{d}}{\mathrm{d}t}E[H] = E\left[\frac{\partial V}{\partial t} - \frac{\partial \boldsymbol{A}}{\partial t}\cdot\boldsymbol{b} - \frac{\nu}{2}\nabla\cdot\frac{\partial \boldsymbol{A}}{\partial t}\right]$$

in analogy with the classical relationship

$$\dot{H} = \frac{\partial V}{\partial t} - \frac{\partial \boldsymbol{A}}{\partial t}\cdot\dot{\boldsymbol{q}}$$

where the expectation is defined in the usual way by

$$E[f] = \int_{R^3} f(\boldsymbol{q},t)\rho(\boldsymbol{q},t)\,\mathrm{d}\boldsymbol{q}.$$

We make some use of the identity

$$\frac{\mathrm{d}}{\mathrm{d}t}E[f] = E\left[\frac{\partial f}{\partial t} + \boldsymbol{v}\cdot\nabla f\right]$$

obtained by an integration by parts argument for suitable ρ in the following. By calculation we have

$$\frac{\partial H}{\partial t} = \frac{\partial V}{\partial t} - \frac{\partial \boldsymbol{A}}{\partial t}\cdot\boldsymbol{b} - \frac{\nu}{2}\nabla\cdot\frac{\partial \boldsymbol{A}}{\partial t} + \frac{\partial \boldsymbol{b}}{\partial t}\cdot(\boldsymbol{p} - m\boldsymbol{b} - \boldsymbol{A}) - \frac{m\nu}{2}\nabla\cdot\frac{\partial \boldsymbol{b}}{\partial t} + \boldsymbol{b}\cdot\frac{\partial \boldsymbol{p}}{\partial t} + \frac{\nu}{2}\nabla\cdot\frac{\partial \boldsymbol{p}}{\partial t}.$$

We have to choose $\boldsymbol{v}$ and $\boldsymbol{p}$ such that

$$E\left[\frac{\partial \boldsymbol{b}}{\partial t}\cdot(\boldsymbol{p} - m\boldsymbol{b} - \boldsymbol{A}) - \frac{m\nu}{2}\nabla\cdot\frac{\partial \boldsymbol{b}}{\partial t} + \boldsymbol{b}\cdot\frac{\partial \boldsymbol{p}}{\partial t} + \frac{\nu}{2}\nabla\cdot\frac{\partial \boldsymbol{p}}{\partial t} + \boldsymbol{v}\cdot\nabla H\right] = 0.$$

Assuming that $\exp(2R)$ decays fast enough to ensure that we can integrate by parts and ignore boundary terms we transform the above into

$$E\left[\frac{\partial \boldsymbol{b}}{\partial t}\cdot(\boldsymbol{p} - \boldsymbol{A} - m\boldsymbol{v}) + \boldsymbol{v}\cdot\left(\frac{\partial \boldsymbol{p}}{\partial t} + \nabla H\right)\right] = 0.$$

We simply choose $m\boldsymbol{v} = \boldsymbol{p} - \boldsymbol{A}$ and $\partial\boldsymbol{p}/\partial t = -\nabla H$ to give us the equality

$$\frac{\mathrm{d}}{\mathrm{d}t}E[H] = E\left[\frac{\partial V}{\partial t} - \boldsymbol{b}\cdot\frac{\partial \boldsymbol{A}}{\partial t} - \frac{\nu}{2}\nabla\cdot\frac{\partial \boldsymbol{A}}{\partial t}\right].$$

Now observe that if we set $\boldsymbol{p} = m\nu\nabla S$ for some real-valued scalar function S to ensure invariance of $\boldsymbol{p}$ we have

$$m\boldsymbol{v} = m\nu\nabla S - \boldsymbol{A} \quad \text{and} \quad m\nu\frac{\partial S}{\partial t} = -H.$$

The partial differential equations for R and S are thus, after some tidying,

$$-\frac{\partial R}{\partial t} = (\nu\nabla S - m^{-1}\boldsymbol{A})\cdot\nabla R + \tfrac{1}{2}\nabla\cdot(\nu\nabla S - m^{-1}\boldsymbol{A})$$

$$-m\nu\frac{\partial S}{\partial t} = \frac{1}{2m}(m\nu\nabla S - \boldsymbol{A})\cdot(m\nu\nabla S - \boldsymbol{A}) - \frac{m\nu^2}{2}(\nabla R\cdot\nabla R + \Delta R) + V.$$

If we now introduce $\psi = \exp(R + \mathrm{i}S)$ we combine these two equations to give

$$\mathrm{i}m\nu\frac{\partial\psi}{\partial t} = \frac{1}{2m}(\mathrm{i}m\nu\nabla + \boldsymbol{A})\cdot(\mathrm{i}m\nu\nabla + \boldsymbol{A})\psi + V\psi.$$

Note that this is just the Schrödinger equation with $m\nu$ replacing $\hbar$.

4. Conclusion

Given a classical dynamical system we have followed a route analogous to one classical approach in order to obtain a differential equation for the drift in the diffusion and have obtained the Schrödinger equation. Our straightforward approach to obtaining the stochastic Lagrangian does not depend on the use of backward drifts or conditioning into the future and results in a well defined geometric expression. This linear equation enables us to find those functions R and S which define the density ρ and drift b of the diffusion process. It is interesting to note that it is $m\nu$ which arises naturally in our derivation of the Schrödinger equation. One could propose that the effect of the background noise as represented by the $\sqrt{\nu}\,\mathrm{d}\boldsymbol{B}_t$ in the Itô equation for $\boldsymbol{q}_t$ should be in some way inversely proportional to the mass of the particle and choosing $\nu = \hbar/m$ would be a convenient way of accommodating this.

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