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On the drift in stochastic mechanics

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Abstract. For a large class of Hamiltonians we express the stochastic mechanical drift in terms of a solution of the classical equation of motion and comment on the use of Itô equations to study how quantum mechanics approximates classical mechanics.

1. Introduction

We consider the Schrödinger equation for a particle in the presence of both a scalar and vector potential, choosing our units so as to only retain $\hbar$ explicitly:

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \left(\frac{1}{2}(\boldsymbol{p}-\boldsymbol{A})^2 + V\right)\psi$$

where $\boldsymbol{p} \equiv (\hbar/\mathrm{i})\nabla$ and $\psi(\boldsymbol{x},0) = \psi_0(\boldsymbol{x})$. For Hamiltonians that are no more than quadratic in position and momentum we have from the classical theory that the expected value of position $\langle \boldsymbol{q} \rangle$ satisfies the classical Newton equation. If in the above $\boldsymbol{A} = \frac{1}{2}\boldsymbol{B}\wedge\boldsymbol{q}$ and $V = \frac{1}{2}\boldsymbol{q}^{\mathrm{T}}\mathbf{C}^2\boldsymbol{q}$ then we have

$$\langle \ddot{\boldsymbol{q}} \rangle = -\boldsymbol{B}\wedge\langle \dot{\boldsymbol{q}} \rangle - \mathbf{C}^2\langle \boldsymbol{q} \rangle.$$

When one considers other Hamiltonians one obtains an equation of motion for $\langle \boldsymbol{q} \rangle$ which one can believe to be, for small $\hbar$, approximately equivalent to the corresponding Newton equation. For a class of Hamiltonians that are anharmonic, Truman (1975) and Elworthy and Truman (1981) have shown that in a particular sense quantum mechanics tends to classical mechanics as $\hbar$ tends to zero. We explore Nelson's stochastic mechanics (Nelson 1985) with a view towards obtaining better information on how quantum mechanics tends to classical mechanics as $\hbar$ tends to zero. In stochastic mechanics we construct a diffusion process in association with the Schrödinger equation and a particular wavefunction ψ. If $\psi \equiv \exp(R+\mathrm{i}S)$ then the diffusion $\boldsymbol{x}_t$ is governed by the Itô equation

$$\mathrm{d}\boldsymbol{x}_t = [\hbar(\nabla R + \nabla S) - \boldsymbol{A}]\mathrm{d}t + \sqrt{\hbar}\,\mathrm{d}\boldsymbol{B}_t$$

where $\boldsymbol{B}_t$ is a Brownian motion. The density of $\boldsymbol{x}_t$ is $\exp(2R)$ with respect to the usual Lebesgue measure. The diffusion process is continuous, so can we say something about the manner in which $\boldsymbol{x}_t$ tends to $\boldsymbol{q}_{\mathrm{cl}}(t)$ as $\hbar$ tends to zero, where $\boldsymbol{q}_{\mathrm{cl}}(t)$ is some solution of the Newton equation of motion? What can we say about the variance of $\boldsymbol{x}_t$ as $\hbar$ tends to zero or as t tends to infinity? Recall that the variance is difficult to compute from the point of view of the classical approach. To this end we concentrate on clarifying the nature of the drift $\hbar(\nabla R + \nabla S) - \boldsymbol{A}$ in the Itô equation for the diffusion process $\boldsymbol{x}_t$.

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2. The nature of the drift

Let us consider the large class of Hamiltonians that are at most quadratic in position and momentum for which the quantum mechanical propagator is expressible in terms of the classical action alone (Davies 1985). If $G(\boldsymbol{y}, \boldsymbol{x}, t)$ is the propagator for the Schrödinger equation $(\mathrm{i}\hbar\partial/\partial t - H)\psi = 0$ then

$$\psi(\boldsymbol{y}, t) = \int_{R^n} G(\boldsymbol{y}, \boldsymbol{x}, t)\psi_0(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

where $G(\boldsymbol{y}, \boldsymbol{x}, t)$ has the representation

$$(2\pi\mathrm{i}\hbar)^{-n/2}\left|-\partial^2 S_{\mathrm{cl}}(\boldsymbol{y}, \boldsymbol{x}, t)/\partial y^j \partial x^k\right|^{1/2} \exp\left(\mathrm{i}S_{\mathrm{cl}}(\boldsymbol{y}, \boldsymbol{x}, t)/\hbar\right)$$

$S_{\mathrm{cl}}(\boldsymbol{y}, \boldsymbol{x}, t)$ being the classical action for a particle moving from $\boldsymbol{x}$ at time 0 to $\boldsymbol{y}$ at time t. We consider t sufficiently small to ensure that there is but one classical path between $\boldsymbol{x}$ and $\boldsymbol{y}$. For this particular class of Hamiltonians the term preceding the exponent is independent of $\boldsymbol{x}$ and $\boldsymbol{y}$. We choose the wavefunction $\psi_0(\boldsymbol{x})$ to be

$$\psi_0(\boldsymbol{x}) = N^{-1}\exp\left(-\Omega(\boldsymbol{x} - \boldsymbol{\mu})^2/2\hbar + \mathrm{i}\boldsymbol{v}\cdot\boldsymbol{x}/\hbar\right)$$

where the constant N ensures that the wavefunction is normalised in $L^2(R^n)$ so as to have the quantum mechanical representation of a particle with position $\boldsymbol{\mu}$ and canonical momentum $\boldsymbol{v}$. It must be stated that for this class of Hamiltonians one can by dint of sheer hard work calculate exactly the expressions to be obtained herein. One will not, however, obtain their nature as will be demonstrated when we consider two simple examples. We now proceed to calculate the exponent of $\psi(\boldsymbol{y}, t)$, as this will give us the drift. The calculation is straightforward but one must take advantage of the fact that $S_{\mathrm{cl}}(\boldsymbol{y}, \boldsymbol{x}, t)$ is no more than quadratic in $\boldsymbol{y}$ and $\boldsymbol{x}$. We express S_{cl} in terms of $\boldsymbol{q}_{\mathrm{cl}}(t)$, which is the classical path satisfying $\boldsymbol{q}_{\mathrm{cl}}(0) = \boldsymbol{\mu}$ and $\boldsymbol{p}_{\mathrm{cl}}(0) = \boldsymbol{v}$, to get the expression

$$\begin{aligned} S_{\mathrm{cl}}(\boldsymbol{y}, \boldsymbol{x}, t) = {} & S_{\mathrm{cl}}(\boldsymbol{q}_{\mathrm{cl}}(t), \boldsymbol{\mu}, t) - \boldsymbol{v}^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{\mu}) + \boldsymbol{p}_{\mathrm{cl}}(t)^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t)) \\ & + \tfrac{1}{2}\left[(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))^{\mathrm{T}}\mathbf{S}_{yy}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t)) + 2(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))^{\mathrm{T}}\mathbf{S}_{xy}^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{\mu})\right. \\ & \left. + (\boldsymbol{x} - \boldsymbol{\mu})^{\mathrm{T}}\mathbf{S}_{xx}(\boldsymbol{x} - \boldsymbol{\mu})\right]. \end{aligned}$$

We have used the notation $(\mathbf{S}_{yy})_{jk} = \partial^2 S_{\mathrm{cl}}/\partial y^j \partial y^k$, etc. Substituting $\boldsymbol{z}$ for $\boldsymbol{x} - \boldsymbol{\mu}$, the exponent in the integrand for calculating $\psi(\boldsymbol{y}, t)$ becomes

$$\begin{aligned} & (\mathrm{i}/\hbar)\left[S_{\mathrm{cl}}(\boldsymbol{q}_{\mathrm{cl}}(t), \boldsymbol{\mu}, t) + \boldsymbol{p}_{\mathrm{cl}}(t)^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t)) + \boldsymbol{v}^{\mathrm{T}}\boldsymbol{\mu} + \tfrac{1}{2}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))^{\mathrm{T}}\mathbf{S}_{yy}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))\right] \\ & \qquad + \boldsymbol{z}^{\mathrm{T}}\left[(-\Omega/2\hbar)I + (\mathrm{i}/2\hbar)\mathbf{S}_{xx}\right]\boldsymbol{z} + (\mathrm{i}/\hbar)\left[\mathbf{S}_{xy}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))\right]^{\mathrm{T}}\boldsymbol{z}. \end{aligned}$$

After performing the integration in $\boldsymbol{z}$ we are left with the exponent in $\psi(\boldsymbol{y}, t)$ as

$$\begin{aligned} & (\mathrm{i}/\hbar)\left[S_{\mathrm{cl}}(\boldsymbol{q}_{\mathrm{cl}}(t), \boldsymbol{\mu}, t) + \boldsymbol{p}_{\mathrm{cl}}(t)^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t)) + \boldsymbol{v}^{\mathrm{T}}\boldsymbol{\mu} + \tfrac{1}{2}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))^{\mathrm{T}}\mathbf{S}_{yy}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))\right] \\ & \qquad + (1/2\hbar)\left[\mathbf{S}_{xy}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))\right]^{\mathrm{T}}\left(-\Omega I + \mathrm{i}\mathbf{S}_{xx}\right)^{-1}\left[\mathbf{S}_{xy}(\boldsymbol{y} - \boldsymbol{q}_{\mathrm{cl}}(t))\right]. \end{aligned}$$

Noting that

$$\left(-\Omega I + \mathrm{i}\mathbf{S}_{xx}\right)^{-1} = \left(\Omega^2 I + \mathbf{S}_{xx}^2\right)^{-1}\left(-\Omega I - \mathrm{i}\mathbf{S}_{xx}\right)$$

and taking the gradient of the above with respect to y shows that the drift $(\hbar(\nabla R + \nabla S) - A)$ can be written as

$$p_{\mathrm{cl}}(t) - A(y, t) + [\mathbf{S}_{yy} - \mathbf{S}^{\mathrm{T}}_{xy}(\Omega^2 I + \mathbf{S}^2_{xx})^{-1}(\Omega I + \mathbf{S}_{xx})\mathbf{S}_{xy}](y - q_{\mathrm{cl}}(t))$$

which simplifies to

$$\dot{q}_{\mathrm{cl}}(t) + (\mathbf{M} - \mathbf{A})(y - q_{\mathrm{cl}}(t))$$

since A is assumed to be linear in its spatial argument and $p = \dot{q} + A$. We have introduced $\mathbf{M}$ as a short notation for a real symmetric time-dependent matrix. We may now write the Itô equation for the diffusion process associated with $\psi(y, t)$ as

$$\mathrm{d}(y_t - q_{\mathrm{cl}}(t)) = (\mathbf{M} - \mathbf{A})(y_t - q_{\mathrm{cl}}(t))\,\mathrm{d}t + \sqrt{\hbar}\,\mathrm{d}B_t.$$

Using $\mathrm{d}(X^2) = 2X\mathrm{d}X + (\mathrm{d}X)^2$ gives us immediately

$$\mathrm{d}(y_t - q_{\mathrm{cl}}(t))^2 = 2(y_t - q_{\mathrm{cl}}(t))^{\mathrm{T}}(\mathbf{M} - \mathbf{A})(y_t - q_{\mathrm{cl}}(t))\,\mathrm{d}t + n\hbar\,\mathrm{d}t + 2\sqrt{\hbar}\,\mathrm{d}B^{\mathrm{T}}_t(\mathbf{M} - \mathbf{A})(y_t - q_{\mathrm{cl}}(t)).$$

Notice that from Nelson's stochastic mechanics the natural object to study is $y_t - q_{\mathrm{cl}}(t)$. The Itô equations above also show that $\langle y_t - q_{\mathrm{cl}}(t)\rangle = 0$ and further that

$$\dot{f}(t) \leq n\hbar + 2f\lambda_{\min}(\mathbf{M} - \mathbf{A})$$

where $f(t) = \langle (y - q_{\mathrm{cl}}(t))^2\rangle$ and $\lambda_{\min}(\mathbf{M} - \mathbf{A})$ is the minimum eigenvalue of $\mathbf{M} - \mathbf{A}$. We appear to have obtained a differential equation for the variance of y_t but this is not quite so.

3. Two cautionary examples

3.1. The free particle in one dimension

Calculating from first principles or following the scheme above leads us to the Itô equation

$$\mathrm{d}(y_t - \mu - vt) = \frac{\Omega(\Omega t - 1)}{1 + \Omega^2 t^2}(y_t - \mu - vt)\,\mathrm{d}t + \sqrt{\hbar}\,\mathrm{d}B_t.$$

Observe that $\langle y\rangle = \mu + vt$ as expected but the variance of y_t increases constantly after a preliminary initial decrease in accord with any quantum mechanical approach.

3.2. The harmonic oscillator in one dimension

Consider the Hamiltonian $H = -\frac{1}{2}\hbar^2\Delta + \frac{1}{2}\omega^2 x^2$. Calculating from first principles or from using the exact form of S_{cl} (Davies 1985) we arrive at the Itô equation

$$\mathrm{d}(y_t - q_{\mathrm{cl}}(t)) = \omega\frac{-\omega\Omega s - \omega^2 c + c(\Omega^2 s^2 + \omega^2 c^2)}{s(\Omega^2 s^2 + \omega^2 c^2)}(y_t - q_{\mathrm{cl}}(t))\,\mathrm{d}t + \sqrt{\hbar}\,\mathrm{d}B_t$$

where $s = \sin\omega t$ and $c = \cos\omega t$. This expression simplifies to the following, on setting $\alpha = \omega/\Omega$:

$$\mathrm{d}(y_t - \boldsymbol{q}_{\mathrm{cl}}(t)) = -\omega\frac{\alpha + (\alpha^2 - 1)cs}{s^2 + \alpha^2 c^2}(y_t - \boldsymbol{q}_{\mathrm{cl}}(t))\,\mathrm{d}t + \sqrt{\hbar}\,\mathrm{d}\boldsymbol{B}_t.$$

It is this simple example which illustrates an inherent problem. For the case of $\alpha = 1$ we have

$$\langle (y - \boldsymbol{q}_{\mathrm{cl}}(t))^2 \rangle = \frac{\hbar}{2\omega}(1 + \mathrm{e}^{-2\omega t})$$

which shows that the variance tends to a small positive constant as t tends to infinity. We always have $\langle (y - \boldsymbol{q}_{\mathrm{cl}}(t))^2 \rangle \sim \hbar$ for finite t. The main problem is that for α substantially different from 1 we have no definite sign for $[\alpha + (\alpha^2 - 1)cs]/(s^2 + \alpha^2 c^2)$ and so we have no tight control of the variance. It may become quite large for certain times t. Note that one could have obtained the variance exactly from first principles. The purpose of this study is to try and lay the foundations for the study of problems which cannot be tackled in a direct way.

4. Conclusion

By employing the methods of classical mechanics we have exhibited the nature of the drift in Nelson's stochastic mechanics showing clearly how the classical velocity is built in for a wide range of Hamiltonians, namely

$$\boldsymbol{b}(y_t, t) = \dot{\boldsymbol{q}}_{\mathrm{cl}}(t) + (\mathbf{M} - \mathbf{A})(y_t - \boldsymbol{q}_{\mathrm{cl}}(t)).$$

We have shown how one may employ the Itô equations derived to calculate the variance of y_t. We have shown how one ought to proceed in anharmonic potentials but have observed that there are problems, specifically the lack of positive definiteness in the matrix $\mathbf{M} - \mathbf{A}$ which plays such a central role. If one considers using the semiclassical method of expressing the quantum mechanical propagator in terms of a Feynman path integral (Truman 1975) one runs into the incompatibility of the classical path used herein and the natural classical path from the path integral point of view. If one pursues the calculations further one obtains a highly unpleasant path integral which is not trivial to compute. I believe that the methods expounded herein would be useful in more general problems for small time t only.

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