The diffusion equation and the principle of minimum Fisher information

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Abstract

It is shown that the diffusion equation and its adjoint (time reversed) equation can be derived with only a few assumptions, using an information-theoretic approach based on the principle of minimum Fisher information.

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I. INTRODUCTION

The derivation of the diffusion equation from a fixed end-point variational principle is well known [1]. The Lagrangian that is normally used leads simultaneously to two equations for two real functions: the diffusion equation for a function $\psi$, and its adjoint (time reversed) equation for a function $\psi^*$. This Lagrangian is usually introduced formally, without physical justification (consider the following quote from Ref. [1]: “The introduction of the mirror-image field $\psi^*$, in order to set up a Lagrange function from which to obtain the diffusion equation, is probably too artificial a procedure to expect to obtain much of physical significance from it”). We wish to show that this Lagrangian results from applying an information-theoretic approach to the solution of the following interpolation problem.

Consider an experiment, where the probability density $\rho(x,t)$ and the average velocity field $v(x,t)$ of a cloud of particles of mass $m$ is measured at times $t_0$ and $t_1$ (for simplicity, we consider only motion in one dimension). Assume that $\rho$ satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) = 0. \tag{1}$$

Without additional assumptions regarding the dynamics of the system, the problem of determining the probability density and velocity field at times $t$ (where $t_0 < t < t_1$) can not be solved, since there are an infinite number of probability densities and velocity fields that will interpolate between the values measured at times $t_0$ and $t_1$. However, we would still like to find best estimates of $\rho$ and $v$, perhaps by adding some assumptions about the physical
processes that determine the motion of the cloud of particles, and by using some principle
of inference to select the most likely probability distribution that might describe its evolu-
tion. The main result of this paper is to show that the dynamics of such a system will be
determined uniquely by the diffusion equation and its adjoint equation,
\[
\frac{\partial \psi}{\partial t} = \frac{D}{2m} \frac{\partial^2 \psi}{\partial x^2},
\]
(2)
\[-\frac{\partial \psi^*}{\partial t} = \frac{D}{2m} \frac{\partial^2 \psi^*}{\partial x^2},
\]
(3)
(where \(\psi\) and \(\psi^*\), defined by eqs. (13) and (14), are real functions of \(\rho\) and \(\sigma\), and \(D/2m\) is
the diffusion constant) provided we make the following two assumptions about the system:
that the velocity field can be derived from a potential function \(\sigma(x,t)\), according to
\[
v = \frac{1}{m} \frac{\partial \sigma}{\partial x},
\]
(4)
and that the probability density \(\rho\) that interpolates between times \(t_0\) and \(t_1\) is the one that
minimizes the Fisher information \(I\) associated with \(\rho\), which we define by (see Appendix A)
\[
I = \frac{1}{m} \int_{t_0}^{t_1} \int_{-\infty}^{+\infty} \frac{1}{\rho} \left( \frac{\partial \rho}{\partial x} \right)^2 \, dx \, dt.
\]
(5)
The first assumption is equivalent to introducing a particular physical model, in which the
motion of the cloud of particles corresponds to that of a fluid with no vorticity. The second
assumption is an information-theoretical assumption.

II. DERIVATION OF THE DIFFUSION EQUATION FROM A VARIATIONAL
PRINCIPLE

Eqs. (1) and (4) lead to the continuity equation
\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left( \rho \frac{1}{m} \frac{\partial \sigma}{\partial x} \right) = 0.
\]
(6)
Eq. (3) can be derived from the Lagrangian \(L_{CL}\) by fixed end-point variation with respect
to \(\sigma\).


\[ L_{CL} = -\int_{t_0}^{t_1} \int_{-\infty}^{+\infty} \rho \left( \frac{\partial \sigma}{\partial t} + \frac{1}{2m} \left( \frac{\partial \sigma}{\partial x} \right)^2 \right) dx dt. \]  

(7)

Note also that fixed end-point variation with respect to \( \rho \) leads trivially to the Hamilton-Jacobi equation,

\[ \frac{\partial \sigma}{\partial t} + \frac{1}{2m} \left( \frac{\partial \sigma}{\partial x} \right)^2 = 0. \]  

(8)

Therefore, variation of \( L_{CL} \) with respect to both \( \rho \) and \( \sigma \) leads to the equations of motion for a classical ensemble, eqs. (6) and (8). There is still considerable freedom in the choice of probability density that can be used to describe the system, since it is only subject to eq. (6). To derive the diffusion equation and its adjoint, we need to restrict the choice of probability densities using the principle of minimum Fisher information. We consider therefore the Lagrangian \( L_D \),

\[ L_D = -\int_{t_0}^{t_1} \int_{-\infty}^{+\infty} \rho \left\{ \frac{\partial \sigma}{\partial t} + \frac{1}{2m} \left( \frac{\partial \sigma}{\partial x} \right)^2 - \frac{D^2}{4} \frac{1}{\rho^2} \left( \frac{\partial \rho}{\partial x} \right)^2 \right\} dx dt. \]  

(9)

The Lagrangian \( L_D \) equals \( L_{CL} \) plus an additional term proportional to the Fisher information \( I \),

\[ L_D = L_{CL} + \frac{1}{2} \frac{D^2}{4} I. \]  

(10)

Fixed end point variation of \( L_D \) with respect to \( \sigma \) leads once more to eq. (6), while variation with respect to \( \rho \) leads to a modified Hamilton-Jacobi equation that includes a term \( Q \) which is of the form of Bohm’s quantum potential [2] (but notice that it appears here within the context of a classical theory),

\[ \frac{\partial \sigma}{\partial t} + \frac{1}{2m} \left( \frac{\partial \sigma}{\partial x} \right)^2 + Q = 0 \]  

(11)

with

\[ Q = -\frac{D^2}{4} \left[ \frac{1}{\rho^2} \left( \frac{\partial \rho}{\partial x} \right)^2 - 2 \frac{\rho}{\rho} \left( \frac{\partial^2 \rho}{\partial x^2} \right) \right]. \]  

(12)

Eqs. (6) and (11) are identical to eqs. (2) and (3) provided we set
\[ \psi = \sqrt{\rho e^{\sigma/D}}, \quad (13) \]
\[ \psi^* = \sqrt{\rho e^{-\sigma/D}}. \quad (14) \]

It can be shown (see Appendix B) that the Fisher information \( I \) increases when \( \rho \) is varied while \( \sigma \) is kept fixed. Therefore, the solution derived here is the one that minimizes the Fisher information for a given \( \sigma \).

III. CONNECTION TO BROWNIAN MOTION

Although \( \psi \) is a solution of the diffusion equation, it will not correspond in general to the case of Brownian motion. Here, \( \psi = \sqrt{\rho e^{\sigma/D}} \) is proportional to the square root of a probability distribution, while in Brownian motion the probability distribution \( \rho \) is the function that satisfies the diffusion equation. The \( \psi \) that we have derived here is essentially the “wave function” of Euclidean quantum mechanics \[3\].

The case of Brownian motion corresponds to a particular solution of eqs. (6) and (11), one for which
\[ \sigma_{BM} = \frac{D}{2} \ln \rho. \quad (15) \]

In this case, the velocity field then takes the form
\[ v_{BM} = \frac{D}{2m} \frac{\partial \ln \rho}{\partial x}. \quad (16) \]

Eq. (16) is known as the osmotic equation, and \( v_{BM} \) is the osmotic velocity. If we substitute \( \sigma_{BM} \) into eqs. (13) and (14), the “wave functions” become
\[ \psi_{BM} = \rho \quad (17) \]
\[ \psi_{BM}^* = 1 \quad (18) \]

which solve eqs. (2) and (3) provided the probability density \( \rho \) is a solution of the diffusion equation. One can also check that eqs. (6) and (11) both reduce to
\[
\frac{\partial \rho}{\partial t} + \frac{D}{2m} \frac{\partial^2 \rho}{\partial x^2} = 0 \tag{19}
\]

when eq. (15) holds.

**IV. DISCUSSION**

It has been shown that the diffusion equation and its adjoint (time reversed) equation can be derived using an information-theoretic approach that is based on the principle of minimum Fisher information. In the information-theoretic approach followed here, the emphasis is on using the principle of minimum Fisher information to complement a physical picture derived from a particular hydrodynamical model of the system. Variation of the Lagrangian (9) can be interpreted as the minimization of the Fisher information subject to the constraint that the probability density satisfy the continuity equation (6), which arises naturally in the hydrodynamical model. An alternative approach to the diffusion equation that also uses minimum Fisher information can be found in Ref. [4]. This derivation, however, differs from the present one in two crucial respects; in particular, the equation is not derived from a Lagrangian, and the derivation does not make reference to the hydrodynamical model.

The approach followed here provides a physically well motivated derivation of the diffusion equation which distinguishes between physical and information-theoretical assumptions. A similar approach leads to the Schrödinger [5] and Pauli [6] equations.

**V. APPENDIX A**

Let \( \mu \) be a measure defined on \( \mathbb{R}^n \), let \( P(y^i) \) be a probability density with respect to \( \mu \) which is a function of \( n \) continuous parameters \( y^i \), and let \( P(y^i + \Delta y^i) \) be the density that results from a small change in the \( y^i \). Expand the \( P(y^i + \Delta y^i) \) in a Taylor series, and calculate the cross-entropy up to the first non-vanishing term,

\[
\int P(y^i + \Delta y^i) \ln \frac{P(y^i + \Delta y^i)}{P(y^i)} d\mu(y^i) \approx \frac{1}{2} \sum_{j,k}^n \left[ \int \frac{1}{P(y^i)} \frac{\partial P(y^i)}{\partial y^j} \frac{\partial P(y^i)}{\partial y^k} d\mu(y^i) \right] \Delta y^j \Delta y^k \tag{20}
\]
The terms in square brackets are the elements of the Fisher information matrix (while this is not the most general definition of the Fisher information matrix, it is one that applies to the present case [5]. For the general case, see Ref. [7]).

If $P$ is defined over an $n$-dimensional manifold $M$ with (positive) metric $g^{ik}$, there is a natural definition of the amount of information $I$ associated with $P$, which is obtained by contracting the metric $g^{ik}$ with the elements of the Fisher information matrix,

$$I = \sum_{j,k} g^{ik} \int \frac{1}{P} \left( \frac{\partial P}{\partial y^j} \right) \left( \frac{\partial P}{\partial y^k} \right) d\mu(y^i).$$

(21)

In the case where $M$ is the $n + 1$ dimensional extended configuration space $QT$ (with coordinates $\{t, x^1, ..., x^n\}$) of a non-relativistic particle of mass $m$, the natural metric is the one used to define the kinematical line element in configuration space, which is of the form $g^{ik} = \text{diag}(0, 1/m, ..., 1/m)$ [8]. Note that with this metric, it is straightforward to generalize the results of the paper to the case of diffusion in many space dimensions. In particular, we replace the velocity field in eq. (4) by the expression $v^i = g^{ik} \partial \sigma / \partial x^k$, and the Lagrangian in eq. (9) by

$$L_D = -\int \rho \left\{ \frac{\partial \sigma}{\partial t} + \frac{1}{2} \sum_{j,k} g^{ik} \left[ \frac{\partial \sigma}{\partial x^i} \frac{\partial \sigma}{\partial x^k} - \frac{D^2}{4 \rho^2} \frac{\partial \rho}{\partial x^i} \frac{\partial \rho}{\partial x^k} \right] \right\} d^n x dt.$$  

(22)

In the case of one time and one space dimension, eq.(21) reduces to eq. (5).

To express $I$ in units of energy, we need to introduce a conversion factor with units of action squared and multiply eq. (5) by this factor. In the case of the diffusion process, we can set the conversion factor proportional to $D^2$, although it is also possible to introduce a universal constant of action, such as $\hbar$, and set the conversion factor proportional to $\hbar^2$.

VI. APPENDIX B

We want to examine the extremum obtained from the fixed end-point variation of the Lagrangian $L_D$. In particular, we wish to show the following: given $\rho$ and $\sigma$ that satisfy eqs. (4) and (11), a small variation of the probability density $\rho(x, t) \rightarrow \rho(x, t)' = \rho(x, t) + \epsilon \delta \rho(x, t)$ for fixed $\sigma$ will lead to an increase in $L_D$, as well as an increase in the Fisher information $I$. 7
We assume fixed end-point variations ($\delta \rho = 0$ at the boundaries), and variations $\epsilon \delta \rho$ that are well defined in the sense that $\rho'$ will have the usual properties required of a probability distribution (such as $\rho' > 0$ and normalization).

Let $\rho \to \rho' = \rho + \epsilon \delta \rho$. Since $\rho$ and $\sigma$ are solutions of the variational problem, the terms linear in $\epsilon$ vanish. If we keep terms up to order $\epsilon^2$, we find that

$$\Delta L_D \equiv L_D(\rho', \sigma) - L_D(\rho, \sigma) = \epsilon^2 \frac{D^2}{8m} \int \int \left\{ \frac{(\delta \rho)^2}{\rho^3} \left( \frac{\partial \rho}{\partial x} \right)^2 - \frac{2\delta \rho}{\rho^2} \left( \frac{\partial \rho}{\partial x} \right) \left( \frac{\partial \delta \rho}{\partial x} \right) + \frac{1}{\rho} \left( \frac{\partial \delta \rho}{\partial x} \right)^2 \right\} \, dx \, dt + O(\epsilon^3). \quad (23)$$

Using the relation

$$\frac{\partial}{\partial x} \left( \frac{\delta \rho}{\rho} \right) = \frac{1}{\rho} \frac{\partial \delta \rho}{\partial x} - \frac{1}{\rho^2} \frac{\partial \rho}{\partial x} \delta \rho, \quad (24)$$

we can write $\Delta L_D$ as

$$\Delta L_D = \epsilon^2 \frac{D^2}{8m} \int \int \rho \left[ \frac{\partial}{\partial x} \left( \frac{\delta \rho}{\rho} \right) \right]^2 \, dx \, dt + O(\epsilon^3), \quad (25)$$

which shows that $\Delta L_D > 0$ for small variations, and therefore the extremum of $\Delta L_D$ is a minimum. Furthermore, since $\Delta L_D \sim D^2$, it is the Fisher information term $I$ in the Lagrangian $\Delta L_D$ that increases, and the extremum is also a minimum of the Fisher information.
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