A Unified View of Transport Equations

J.A. Secrest\textsuperscript{1}, J.M. Conroy\textsuperscript{2} and H.G. Miller\textsuperscript{2}

\textsuperscript{1}Department of Physics and Astronomy, Georgia Southern University, Armstrong Campus, Savannah, Georgia, USA and
\textsuperscript{2}Department of Physics, State University of New York at Fredonia, Fredonia, New York, USA

(Dated: June 18, 2019)

Abstract

Distribution functions of many static transport equations are found using the Maximum Entropy Principle. The equations of constraint which contain the relevant dynamical information are simply the low-lying moments of the distributions. Systems subject to conservative forces have also been considered.
I. INTRODUCTION

Transport phenomena is the description of how physical quantities such as the number of particles or the energy flow through a medium. In general these phenomena are described by various differential equations, for example, the Boltzmann equation, diffusion equation, and the advection equation \[1–3\]. In the simplest case the solutions of many of these equations, i.e. the distribution functions, \( \rho(x) \), have one thing in common in that they are simple Gaussian distributions which do not change as a function of time. At any given point in time or in the static case, these distributions are uniquely determined by knowledge of at most two moments. This strongly suggests that the relevant dynamical information to be included is contained in the moments. Rather than model these phenomena by constructing a differential equation in each case one can use the Maximum Entropy Principle (MEP) \[4, 5\] where the dynamics are contained in the equations of constraint.

In the static case the MEP requires that the information entropy, \( S(\rho) \), satisfies the equation

\[
\delta \rho S(\rho) = 0 \tag{1}
\]

subject to the relevant equations of constraint

\[
Tr(\rho(x) O_i(x)) = r_i. \tag{2}
\]

Classically

\[
S(\rho) = -\int_{-\infty}^{\infty} \rho(x) \ln \frac{\rho(x)}{\rho_0(x)} \, dx \tag{3}
\]

and \( \rho_0(x) \) is an invariant measure. The solution to the above equations is given by

\[
\rho(x) = \rho_0(x) e^{\sum_{i=0}^{\infty} \lambda_i O_i(x)} \tag{4}
\]

and the Lagrange multipliers, \( \lambda_i \), are determined from the equations of constraint.

In the simplest cases, as we shall show, the relevant choice for \( O_i(x) \) is given by the lowest moments of \( x \)

\[
O_i(x) = x^i \tag{5}
\]

for \( i = 0, 1, 2 \) as this will ultimately yield Gaussian distributions since the \( i = 1 \) component will not contribute.
Furthermore if the system is acted on by an external conservative force derivable from a potential, \( K(x) = -\frac{\partial u(x)}{\partial x} \), such that

\[
\frac{dx}{dt} = K(x),
\]

the accompanying Liouville equation is of the form [6]

\[
J(x) = \rho(x)K(x)
\]

where the current \( J(x) \) satisfies the continuity equation

\[
\frac{\partial \rho(x)}{\partial t} + \nabla \cdot J(x) = 0.
\]

In the static case the current \( J(x) \) is constant. Since \( \rho(x) \rightarrow 0 \) as \( x \rightarrow \pm \infty \) the constant must be 0. Hence

\[
\rho(x)\frac{\partial u(x)}{\partial x} = 0.
\]

Integrating by parts where the initial potential \( u(x_0) = 0 \) yields

\[
\rho(x)u(x) = \int_{x_0}^{x} \frac{\partial \rho(x)}{\partial x} u(x) dx
\]

or

\[
Tr[\rho(x)u(x)] = Tr \left[ \int_{x_0}^{x} \frac{\partial \rho(x)}{\partial x} u(x) dx \right],
\]

which is the proper form for an equation of constraint (see Eq.(2)).

Hence the general form of the distribution functions associated with many of the well known transport equations is given by

\[
\rho(x) = e^{\sum_{i=0}^{2} \lambda_i x^i + \lambda_3 u(x)}
\]

with \( i = 0, 1, 2 \). The values of the Lagrange multipliers are determined by the relevant equations of constraint which contain the information about the particular dynamics involved.

II. EXAMPLES

In this section the use of the MEP for solving transport phenomena equations is demonstrated through a number of examples. The analytic solution is known in each of the following examples. In practice, the necessary constraints would be determined experimentally.
and applied to the MEP general solution. For example, the second spatial time-dependent moment of the diffusion equation studied below can be determined by measuring the diffusion constant and invoking the Einstein relation as discussed below. Another example would be to determine the velocity moments by measuring the momentum distributions. In the following examples one spatial dimension is considered, though the MEP can be extended to higher dimensions.

A. Advection Equation

The advection equation is a hyperbolic partial differential equation of the form

\[
\frac{\partial \rho(x, t)}{\partial t} = -v \frac{\partial \rho(x, t)}{\partial x}
\]

that describes how a scalar field density \( \rho \) is swept along (advected) by a bulk flow of constant speed \( v \). The position \(-\infty < x < \infty\), the time \( 0 < t < \infty \), and the velocity field \( v \) are nonzero. Examples of where the advection equation is used are modeling automobile traffic, blood flow through a capillary, and salinity propagation in the ocean.

A particular solution to this equation is

\[
\rho(x, t) = e^{-\left(x - vt\right)^2}.
\]

The moments calculated using the actual solution (which would be experimentally determined) are:

\[
r_0 = \int_{-\infty}^{\infty} e^{\left(x - vt\right)^2} \, dx = \sqrt{\pi},
\]

\[
r_1 = \int_{-\infty}^{\infty} xe^{\left(x - vt\right)^2} \, dx = \sqrt{\pi} vt,
\]

and

\[
r_2 = \int_{-\infty}^{\infty} x^2 e^{\left(x - vt\right)^2} \, dx = \frac{1}{2} \sqrt{\pi} [1 + 2v^2 t^2].
\]
The moments calculated from the generalized MEP solution seen in Eq. 4 are:

\[
    r_0 = \int_{-\infty}^{\infty} e^{-\lambda_2 x^2 - \lambda_1 x - \lambda_0} dx = e^{-\lambda_0} \left[ \frac{\lambda_1^2}{2(1 + \lambda_2)^{3/2}} \right],
\]

(18)

\[
    r_1 = \int_{-\infty}^{\infty} x e^{-\lambda_2 x^2 - \lambda_1 x - \lambda_0} dx = e^{-\lambda_0} \left[ -\frac{\lambda_1^2}{2(1 + \lambda_2)^{3/2}} \right],
\]

(19)

and

\[
    r_2 = \int_{-\infty}^{\infty} x^2 e^{-\lambda_2 x^2 - \lambda_1 x - \lambda_0} dx = e^{-\lambda_0} \left[ \frac{(2\lambda_2 + \lambda_1^2)^{3/2}}{2(1 + \lambda_2)^{5/2}} \right].
\]

(20)

Equating the moments and solving for the Lagrange multipliers, \( \lambda_0 = (vt)^2 \), \( \lambda_1 = -2vt \), and \( \lambda_2 = 1 \). Substituting these results back into the MEP solution Eq.(4) results in the solution given by Eq.(14).

### B. Diffusion Equation

This choice of the diffusion equation is a linear partial differential equation with a constant diffusion constant \( D \) with the form

\[
    \frac{\partial \rho(x, t)}{\partial t} = D \frac{\partial^2 \rho(x, t)}{\partial x^2}
\]

(21)

that describes how a scalar field density \( \rho \) spreads out as a function of position \( x \) and time \( t \). This equation describes the collective motion of random particles. The same equation also describes heat flow, financial markets and free particles in non-relativistic quantum mechanics. After some time \( t \), the particular solution (where the diffusion constant has been set equal to one) is

\[
    \rho(x, t) = \frac{\sqrt{2\pi\sigma}}{\sqrt{\pi(2\sigma + 4t)}} e^{-\frac{x^2}{2(\sigma + 4t)}}
\]

(22)

with the initial condition that

\[
    \rho_0(x, 0) = e^{\frac{x^2}{2\sigma}}.
\]

(23)

Notice that the MEP solution must require the prefactor due to the initial condition. It will also be discovered that the linear term is zero. In this case,

\[
    \rho = \rho_0 e^{-\lambda_2 x^2 - \lambda_1 x - \lambda_0} = e^{-\frac{(1 + \lambda_2)x^2}{2\sigma} - \lambda_0}. \tag{24}
\]
The moments calculated from the analytic solution (which would be experimentally measured) are:

\[ r_0 = \int_{-\infty}^{\infty} \sqrt{2\pi\sigma} e^{-\frac{x^2}{2\sigma+4t}} = \sqrt{2\pi\sigma} \quad (25) \]

\[ r_1 = \int_{-\infty}^{\infty} x \sqrt{2\pi\sigma} e^{-\frac{x^2}{2\sigma+4t}} = 0 \quad (26) \]

and

\[ r_2 = \int_{-\infty}^{\infty} x^2 \sqrt{2\pi\sigma} e^{-\frac{x^2}{2\sigma+4t}} = \sqrt{2\pi\sigma}(2t+\sigma) \quad (27) \]

The moments calculated from the MEP solution Eq. (4) are:

\[ r_0 = \int_{-\infty}^{\infty} e^{-\left(\frac{1}{2\sigma} + \lambda_2\right)x^2 - \lambda_0} = e^{-\lambda_0} \frac{\sqrt{2\pi}}{2\lambda_2 + \frac{1}{\sigma}} \quad (28) \]

\[ r_1 = \int_{-\infty}^{\infty} x e^{-\left(\frac{1}{2\sigma} + \lambda_2\right)x^2 - \lambda_0} = 0 \quad (29) \]

and

\[ r_2 = \int_{-\infty}^{\infty} x^2 e^{-\left(\frac{1}{2\sigma} + \lambda_2\right)x^2 - \lambda_0} = e^{-\lambda_0} \frac{\sqrt{2\pi}}{(2\lambda_2 + \frac{1}{\sigma})^{\frac{3}{2}}} \quad (30) \]

(31)

Note that the first moment is zero from both calculations, indicating that there is no linear term in the exponent above. Equating the moments and solving for the Lagrange multipliers, it is found that \( e^{-\lambda_0} = \sqrt{\frac{1}{2\sigma+4t}} \) and \( \lambda_2 = -\frac{2t}{2\sigma(2\sigma+4t)} \). Substituting back the solutions for the Lagrange multipliers into Eq. (24) results in the solution given by Eq. (22). In this example, the second spatial moment can be determined from the Einstein-Smoluchowski relation for the diffusion constant \( D \).

C. Fokker-Planck Equation with Logarithmic Potential

The Fokker-Planck Equation is given by

\[ \frac{\partial f(x, t)}{\partial t} = D \left[ \frac{\partial}{\partial x} K(x) - \frac{\partial^2}{\partial x^2} \right] \rho(x, t) \]

where \( \rho(x, t) \) is the probability distribution function, \( K(x) \) is related to the external force acting on the particles, and \( D \) is the diffusion constant. The forcing function is related to a potential function \( u(x) \) measured in units of Boltzmann temperature \( k_B T = 1 \). One choice
for the potential which can be solved for analytically is that of a logarithmic potential:

$$u(x) = -U_0 \ln(|x|/a)$$  \hspace{1cm} (32)

where once again the diffusion constant has been set equal to one. This yields the steady state solution

$$\rho(x) = \frac{U_0 - 1}{2a} \left( \frac{|x|}{a} \right)^{-U_0}.$$  \hspace{1cm} (33)

The zeroth moment and the expectation value of the potential energy were calculated to be

$$r_0 = 2 \int_a^\infty \frac{1}{2a} e^{-U_0 \ln(x/a)} = 1$$  \hspace{1cm} (34)

$$\overline{u(x)} = 2 \int_a^\infty U_0 \ln \left( \frac{x}{a} \right) e^{-U_0 \ln(x/a)}$$

$$= \frac{U_0}{U_0 - 1}.$$  \hspace{1cm} (35)

Determining the zeroth moment and the expectation value of the potential energy using the MEP solution Eq.(12), it is found that

$$r_0 = 2 \int_a^\infty e^{\lambda_0 + \lambda_3 U_0 \ln(x/a)}$$

$$= 2C \int_a^\infty e^{\lambda_3 U_0 \ln(x/a)}$$

$$= \frac{2aC}{1 + \lambda_3 U_0}$$  \hspace{1cm} (36)

$$\overline{u(x)} = 2 \int_a^\infty U_0 \ln \left( \frac{x}{a} \right) e^{\lambda_0 + \lambda_3 U_0 \ln(x/a)}$$

$$= 2C \int_a^\infty U_0 \ln \left( \frac{x}{a} \right) e^{\lambda_3 U_0 \ln(x/a)}$$

$$= \frac{2aCU_0}{(1 + \lambda_3 U_0)^2}.$$  \hspace{1cm} (37)

where the normalization constant has been rewritten as $e^{\lambda_0} = C$. Solving for the MEP solution using the undetermined multipliers $\lambda_0$ and $\lambda_3$ yield the steady state solution Eq.(33).

It is clear that no other moments contribute to constraining of the probability distribution function.

III. CONCLUSIONS

A unified view of transport equations is possible within the framework of MEP. The MEP solution that maximizes the information entropy with respect to the constraints is seen in
Eq. (12). These constraints are typically moments of the distribution function but they may also be constrained by other physical parameters such as a conservative potential. In the case of diffusive phenomena such as Brownian motion, one can determine the temporal evolution of the second spatial moment from measurements of the diffusivity, \( <x^2> = r_2 = 2Dt \).

A general form of the solution of distribution function for various transport phenomena has been found using the MEP. Various low-lying moments have been used as the equations of constraint. This was applied to the advection equation and the diffusion equation. For distributions that are constant in time the time-dependent solutions along with any initial conditions that were specified are used as these constraints. It was shown that the potential energy of a conservative force could be used as a constraint on the distribution function. This was illustrated in determining the steady-state solution to the Fokker-Planck equation with a logarithmic potential. It should be noted that this yields an interesting solution that is ultimately a power-law solution instead of the more frequently encountered exponential-type solutions found with the MEP (though it should be noted that all types of distributions have been determined with MEP). Finally, using this technique to constrain the distribution from the potential opens up a number of different solutions to be found from transport equations that have conservative source terms. Lastly the MEP can be extended to obtain time dependent solutions [10].

[1] T. Bennett, ”Transport by Advection and Diffusion”, Wiley, (2012)
[2] D. L. Powers, ”Boundary Value Problems”, Harcourt Brace Jovanovich, (1972)
[3] G. B. Arfken, H. J. Weber, and F. E. Harris, ”Mathematical Methods for Physicists: A Comprehensive Guide”, Academic Press, (2012)
[4] C. E. Shannon, Bell Syst. Tech. J. 27, 379 (1948)
[5] E. T. Jaynes, Phys. Rev. 106, 620 (1957)
[6] A.R. Plastino and A. Plastino, Physica A, 222 (1995) 347 354
[7] A. Einstein, Ann. der Physik, 17549 (1905)
[8] M. von Smoluchowski, Ann. der Physik, 21 756 (1906)
[9] A. Dechant, E. Lutz, E. Barkai, D. A. Kessler, J Stat Phys, 145, 1524 (2011)
[10] E. D. Malaza, H. G. Miller, A. R. Plastino, F. Solms, Physica A, 265 224 (1999)