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## Modeling spin magnetization transport in a spatially varying magnetic field

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## ABSTRACT

We present a framework for modeling the transport of any number of globally conserved quantities in any spatial configuration and apply it to obtain a model of magnetization transport for spin-systems that is valid in new regimes (including high-polarization). The framework allows an entropy function to define a model that explicitly respects the laws of thermodynamics. Three facets of the model are explored. First, it is expressed as nonlinear partial differential equations that are valid for the new regime of high dipole-energy and polarization. Second, the nonlinear model is explored in the limit of low dipole-energy (semi-linear), from which is derived a physical parameter characterizing separative magnetization transport (SMT). It is shown that the necessary and sufficient condition for SMT to occur is that the parameter is spatially inhomogeneous. Third, the high spin-temperature (linear) limit is shown to be equivalent to the model of nuclear spin transport of Genack and Redfield (1975) [1]. Differences among the three forms of the model are illustrated by numerical solution with parameters corresponding to a magnetic resonance force microscopy (MRFM) experiment (Degen et al., 2009 [2]; Kuehn et al., 2008 [3]; Sidles et al., 2003 [4]; Dougherty et al., 2000 [5]). A family of analytic, steady-state solutions to the nonlinear equation is derived and shown to be the spin-temperature analog of the Langevin paramagnetic equation and Curie's law. Finally, we analyze the separative quality of magnetization transport, and a steady-state solution for the magnetization is shown to be compatible with Fenske's separative mass transport equation (Fenske, 1932 [6]).

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## 1. Introduction

Magnetization transport for a spin-system in a spatially varying magnetic field has been studied theoretically [1] and experimentally [7,8]. High-temperature models of spin magnetization transport, such as that of Genack and Redfield, do not apply for systems with high-polarization. With recent significant enhancements of the technique of *dynamic nuclear polarization* (DNP) [9–11], which has been shown to achieve significant *hyperpolarization*, models that can describe the high-polarization regime in a spatially varying magnetic field are needed.

We present a framework for modeling the transport of any number of globally conserved quantities in any spatial configuration. We then apply it to obtain a model of magnetization transport for spin-systems that is valid in new regimes (including high-polarization). Finally, we analyze the separative quality of the magnetization transport. A particularly useful feature of the

framework is that specifying an entropy density function *completely determines the system model*. Such a function is presented for a spin-system, and its validity is demonstrated by deriving classical models from it, which is justification for using it in new regimes (as we do in Section 3). In Section 2, we introduce the framework. It is general in the sense that it can be applied to systems with any number of globally conserved distributed quantities that evolve over any (smooth) spatial geometry in any number of spatial dimensions. The laws of thermodynamics are included *a priori* such that any specific model based on the framework will be guaranteed to respect all four laws.

In Section 3, we apply the framework by specifying conserved quantities, an entropy function, and a spatial geometry for a spin-system and thereby obtain a new model of magnetization transport in a magnetic field gradient. It accommodates previously unmodeled regimes of high energy and high polarization, such as may develop with DNP. The remainder of the section explores the model in various limits and connects them to previous models.

In Section 4, we analyze the separative quality of magnetization transport, highlighting the parallelism between it and the separative mass transport work that began with Fenske [6]. Magnetization transport in a magnetic field gradient is both

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diffusive and separative, and the latter is of particular interest for technologies that may be enhanced by hyperpolarization, such as magnetic resonance imaging (MRI), nuclear magnetic resonance (NMR) spectroscopy, and magnetic resonance force microscopy (MRFM). DNP has been used to achieve significant hyperpolarization through transferring polarization from electron-spins to nuclear-spins. But DNP is still a slow process, taking tens to thousands of seconds to develop, and it is impeded by magnetic field gradients, which for certain applications (such as MRFM) is undesirable. We consider the feasibility of a different technique in which no polarization is transferred among spin-species, but in which magnetization is concentrated by the phenomenon of *separative magnetization transport* (SMT). We develop the necessary and sufficient conditions for the SMT of a single spin-species—most notably, that the magnetic field must be spatially varying. Taken as a whole, this paper lays the groundwork for an investigation into how the SMT effect might be enhanced to produce hyperpolarization.

## 2. Framework for transport analysis

We will proceed in the coordinate-free language of differential geometry, which allows the laws of thermodynamics to be respected explicitly, regardless of spatial geometry or the number of conserved quantities.

What follows is a necessarily extensive list of definitions and remarks. As we will see, the mathematical rigor of these definitions will enable and greatly simplify the subsequent theoretical development.

The following definitions are the elements from which two propositions are constructed that describe a framework for transport analysis and its adherence to the laws of thermodynamics. In any specific application of the framework, defining the spatial geometry, conserved quantities, entropy function, and a space-time scale will be sufficient to construct a model of transport that respects the laws of thermodynamics from the following definitions (as detailed in Remark 2).

The elements of the framework are defined in the following order:

- (a) the spatial manifold, metric, and coordinates;
- (b) conserved quantities and their local densities;
- (c) the entropy density and thermodynamic potentials;
- (d) Onsager’s kinetic coefficients;
- (e) the current of local quantity densities;
- (f) the continuity equation for local densities; and
- (g) a transport rate tensor and an *ansatz* further specifying the kinetic coefficients.

Proposition 1 will describe how the laws of thermodynamics are satisfied in the definitions and Proposition 2 will assert that the definitions describe a physically valid model of transport. We begin with spatial considerations.

**Definition 1** (*spatial manifold*). Let  $\mathcal{U}$  be a Riemannian (smooth) manifold, which represents the spatial geometry of a macroscopic thermodynamic system. We call  $\mathcal{U}$  the *spatial manifold*. □

For many applications, a Euclidean space<sup>1</sup>  $\mathbb{R}^m$  is an appropriate choice for  $\mathcal{U}$ .

**Remark 1** (*spatial coordinates*). Let  $\varphi : \mathcal{U} \rightarrow \mathbb{R}^m$  be some *local coordinate map*.<sup>2</sup> Typically, we will denote component functions

of  $\varphi$ , defined by  $\varphi(p) = (r^1(p), \dots, r^m(p))$  for some point  $p \in \mathcal{U}$ , as  $(r^1, \dots, r^m)$ . These are called *local spatial coordinates*, and typically denoted  $(r^\alpha)$  (see Fig. 1.) □

By definition, the Riemannian spatial manifold  $\mathcal{U}$  is endowed with a Riemannian metric, which determines the geometry of  $\mathcal{U}$ .

**Definition 2** (*spatial metric*). Let  $g$  be a Riemannian metric<sup>3</sup> on  $\mathcal{U}$ . We call  $g$  the *spatial metric*. □

In local spatial coordinates, the metric is written as

$$g = g_{\alpha\beta} dr^\alpha \otimes dr^\beta. \tag{1}$$

**Definition 3** (*conserved quantities*). Let  $\mathbf{q} \in \mathbb{R}^n$  be the  $n$ -tuple  $\mathbf{q} = (q_1, \dots, q_n)$ , where  $q_i \in \mathbb{R}$  represents a *conserved quantity*. □

**Definition 4** (*standard thermodynamic dual basis*). Let the ordered basis  $(\varepsilon^1, \dots, \varepsilon^n)$  for  $\mathbb{R}^n$  be

$$\varepsilon^1 = (1, 0, \dots, 0), \quad \dots \quad \varepsilon^n = (0, 0, \dots, 1).$$

We call this the *standard thermodynamic dual basis*,<sup>4</sup> and it is often denoted  $(\varepsilon^i)$ . □

In the standard basis, with the *Einstein summation convention*,

$$\mathbf{q} = [q_\varepsilon]_i \varepsilon^i. \tag{2}$$

**Definition 5** (*local quantity density*). Let  $\mathcal{O}^*$  be the set of smooth maps from  $\mathcal{U} \times \mathbb{R}$  (where  $\mathbb{R}$  represents time) to  $V^* \equiv \mathbb{R}^n$  (i.e. for each point in space and time we assign a vector in  $\mathbb{R}^n$ ). Given a vector of conserved quantities  $\mathbf{q}$ , let  $\rho \in \mathcal{O}^*$  represent the local spatial density of each of the conserved quantities  $\mathbf{q}$ , such that

$$\mathbf{q} = \int_{\mathcal{U}} \rho \, dv, \tag{3}$$

where  $dv$  is a volume element of  $\mathcal{U}$ . □

In the standard thermodynamic dual basis  $(\varepsilon^i)$ , we write

$$\rho = [\rho_\varepsilon]_i \varepsilon^i, \tag{4}$$

where each  $[\rho_\varepsilon]_i$  is a function  $[\rho_\varepsilon]_i : \mathcal{U} \times \mathbb{R} \rightarrow \mathbb{R}$ . The mathematical structure of  $\rho$  assigned in the definition is equivalent to a section of the product bundle  $\mathcal{U} \times \mathbb{R} \times V^* \rightarrow \mathcal{U} \times \mathbb{R}$ . Fig. 2 illustrates this description, where copies of  $V^* = \mathbb{R}^n$  correspond to each location in  $\mathcal{U}$ .

We now turn to entropic considerations.

**Definition 6** (*local entropy density*). Let the *local entropy volumetric density function*  $s : V^* \rightarrow \mathbb{R}$  be a function that is nonnegative and concave. □

The restriction of the local entropy density  $s$  to nonnegative functions satisfies the *third law of thermodynamics*. Moreover, we require that  $s$  be concave to allow the Legendre dual relationship that will now be introduced.

At times it is convenient to work with another set of variables called *local thermodynamic potentials*. These are significant because their spatial gradients drive the flow of  $\rho$ .

**Definition 7** (*local thermodynamic potentials*). Let  $\Omega : \mathcal{U} \times \mathbb{R} \rightarrow V$  be defined by the relation

$$\Omega = ds \circ \rho, \tag{5}$$

where the exterior derivative  $d$  is taken with respect to the vector

<sup>3</sup> See [14, p. 23].

<sup>4</sup> Although it is an uncommon practice to introduce a dual basis before a basis, we do so here because the quantities represented by the quantities  $\mathbf{q}$  and  $\rho$  are more naturally—from a physical standpoint—considered dual to the potentials  $\Omega$ . Yet, the quantities naturally arise first in the series of definitions.

<sup>1</sup> See [12, p. 22] and [13, p. 598].

<sup>2</sup> See [13, pp. 15–16, 60–65].

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