

# CONSISTENT MEAN FIELD OPTIMALITY CONDITIONS FOR INTERACTING AGENT SYSTEMS\*

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**Abstract.** We are interested in the derivation of optimality conditions for controlled interacting agent systems. We establish the relation between mean field optimality conditions and the optimality condition of the mean field control problem. This link is important for many recently published articles on control strategies for agent based systems since it establishes the precise relation between multipliers for the individual agents and the probability density distribution of the multipliers in the mean field limit. The relation to different notions of differentiability are also shown.

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**AMS subject classifications.** 82B40; 49J15; 49J20.

## 1. Introduction

Dynamic agent systems have been used recently to describe phenomena different from classical statistical mechanics, see e.g. the recent publications [7, 15, 22, 24]. In many of those descriptions control actions may be applied in order to drive the system towards a desired state using either open, closed loop or a competitive game setting. Of particular interest has been the question of control actions prevailing in the meanfield limit, i.e., in the limit of dynamical systems with infinitely many agents. Many examples have been given in recent literature. We only recall a few results and refer to the references therein for more details. For a Nash game theoretic setting the meanfield limit has been discussed e.g. in [21], and for Stackelberg games in [2, 10]. Closed loop feedback controls have been proposed in [4, 17] and using the additional constraint of sparse controls for example in [11].

In the case of finitely many interacting agents the associated open loop control problem can be solved for example using Pontryagin’s maximum principle (PMP), dynamic programming or the corresponding Hamilton–Jacobi equations. Similarly, open loop control problems with respect to meanfield partial differential equations can be solved using a version of the Lagrange multiplier theorem in infinite dimensional spaces. In this paper we are interested in the relation between both approaches. In particular, we are interested in the corresponding meanfield limit of the optimality conditions arising from the PMP and its relation to the multipliers obtained by the optimization with respect to the partial differential equation. This link is only partially explored so far. Prior work [1, 3–6, 16] on control problems for agent systems applied feedback control techniques to simplify the optimization problem. Typically, the obtained system yields a formulation of the control depending on the current state of the system. Hence, in the aforementioned publications it was not required to consider also the meanfield limit of the corresponding multipliers. However, a formulation of the control as a function of the current state allows to obtain meanfield limits similar to classical kinetic theory. Here, we do not intend to obtain such a closed–loop form of the control, but rather study the meanfield limit to the full optimality system. We study both the meanfield limit

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of optimized agent system as well as the optimized meanfield problem. Furthermore, many results in literature are devoted to control of one-dimensional phase models motivated as models for wealth modeling or opinion formation [19, 23]. Here, we study the case of an arbitrary phase space where simplifications of the particular one-dimensional setting do not hold true any more. In particular, we establish the link of the continuous multiplier and the conditional expectation of the meanfield limit of the optimized agent system.

This paper is organized as follows. In Section 2 we first establish the optimal control system, based on the well known Pontryagin principle, for a system of  $N$  agents, each influenced by agent to agent interaction forces. Assuming sufficient regularity an application of PMP leads to the well-known two point boundary value problem in time for the agent states and a set of  $N$  Lagrange multipliers, augmented by algebraic conditions for an external control variable. Then we proceed to derive a mean field equation for the agent state and its multiplier leading to a multi-variable density distribution. Finally, we derive an effective single agent mean field equation for the probability density of a single agent and the corresponding meanfield Lagrange multipliers under the independently and identically distributed (IID) assumption. In Section 3 we compare this approach to the approach found in the literature. This approach relies to first derive a meanfield equation for the dynamics of an effective single agent and then deriving an optimal control system for the resulting transport equation, again via PMP. We note the obvious difference, which arises from the fact that functional differences are not taken in the space of density functions, but along the manifold of probability densities with integral equal to unity. In Section 4 we discuss the connection between the three models, the ODE model for  $N$  agents, the corresponding joint mean field model for the effective single agent *together with the Lagrange multipliers*, and the PDE optimization model based on optimizing the mean field dynamics. In the Appendix we give a brief review of various other existing approaches to optimizing functionals over manifolds.

## 2. Controlled Interacting Agent Systems

**2.1. Control of an  $N$ - agent system with binary interactions.** We consider controlled dynamics for a set of  $N$  agents, given by

$$\frac{d}{dt}\xi_n = \frac{1}{N} \sum_{m=1}^N p(\xi_n, \xi_m, u), \quad \xi_n(0) = \xi_n^I, \quad n = 1, \dots, N, \quad \xi_n \text{ and } p \in \mathbb{R}^K, \quad n = 1, \dots, N. \quad (2.1)$$

We assume that, in general, the states  $\xi_n = \xi_n(t)$ ,  $n = 1, \dots, N$  are  $K$ - dimensional, i.e.  $\xi_n \in \mathbb{R}^K$ . The mean-field will be considered in the number of particles  $N \rightarrow \infty$  while the dimension of the phase space  $K$  of each particle remains fixed. We also denote by  $\vec{\xi} = (\xi_n)_{n=1}^N \in \mathbb{R}^{KN}$  the vector of all states. We also omit the dependence of  $\xi_n$  and  $u$  on time  $t$  whenever the intention is clear. The initial positions  $\xi_n^I$  are given. Also, we assume  $p: \mathbb{R}^{2K+1} \rightarrow \mathbb{R}$  is at least differentiable in its arguments. For simplicity, we assume  $u = u(t) \in \mathbb{R}$  is the common control for all agents. It is not restrictive to assume  $u \in \mathbb{R}$  and the subsequent results extend to the case  $u \in \mathbb{R}^M$ . The control is chosen to minimize a common objective functional on a time horizon  $T > 0$  given by

$$\int_0^T \frac{1}{N} \sum_{n=1}^N \phi(\xi_n(t), u(t)) dt. \quad (2.2)$$

The function  $\phi: \mathbb{R}^K \times \mathbb{R} \rightarrow \mathbb{R}$  is assumed to be differentiable. In the present formulation  $\phi$  may contain also a regularization term in the control. This is possibly required when discussing existence and uniqueness of the problem (2.2) and (2.1).

EXAMPLE 2.1. In [4] a simple model for opinion formation has been proposed where  $\xi_n \in \mathbb{R}$ . The function  $p$  is then given by  $p(\xi_n, \xi_m, u) = P(\xi_n, \xi_m)(\xi_m - \xi_n) + u$  for a given function  $P: \mathbb{R}^2 \rightarrow \mathbb{R}$  and  $\phi(\xi_n, u) = (\xi_n - z_d)^2 + \frac{1}{2}u^2$  for a given desired state  $z_d$ . Under suitable assumptions on  $p$  and  $\phi$  and using classical results from PMP the optimality conditions to (2.2) and (2.1) are found as saddle point to the Lagrangian given by

$$\frac{1}{N} \sum_{n=1}^N \int_0^T -\mu_n^T \frac{d}{dt} \xi_n dt + \frac{1}{N^2} \sum_{n=1}^N \sum_{m=1}^N \int_0^T \mu_n^T p(\xi_n, \xi_m, u) dt + \frac{1}{N} \sum_{n=1}^N \int_0^T \phi(\xi_n, u) dt. \tag{2.3}$$

Here,  $\vec{\mu} = (\mu_1, \dots, \mu_N)^T \in \mathbb{R}^{NK}$  is the vector of discrete (time-dependent) Lagrange multipliers. The first-order optimality conditions lead to the variational form for any  $n$  and arbitrary perturbations  $\delta \xi_n$

$$\begin{aligned} & \frac{1}{N} \int_0^T \sum_{n=1}^N \delta \xi_n^T \frac{d}{dt} \mu_n + \frac{1}{N^2} \sum_{m=1}^N \sum_{n=1}^N \int_0^T \delta \xi_n^T \partial_1 p(\xi_n, \xi_m, u)^T \mu_n dt \\ & + \frac{1}{N^2} \sum_{m=1}^N \sum_{n=1}^N \int_0^T \delta \xi_m^T \partial_2 p(\xi_n, \xi_m, u)^T \mu_n dt + \frac{1}{N} \sum_{n=1}^N \int_0^T \delta \xi_n^T \nabla_\xi \phi(\xi_n, u) dt = 0. \end{aligned}$$

Here we denote by  $\partial_1 p$  and  $\partial_2 p$  the  $K \times K$  Jacobians with entries  $\partial_1 p(x, y, u)_{jk} = \frac{\partial p_j(x, y, u)}{\partial x_k}$  and  $\partial_2 p(x, y, u)_{jk} = \frac{\partial p_j(x, y, u)}{\partial y_k}$ , respectively. Further,  $\nabla_x \phi(x, u)$  and  $\nabla_u \phi(x, u)$  denotes the gradients of  $\phi$  with respect to  $x$  and  $u$ , respectively. Also, we denote by  $\text{div}_x p(x, y, u) = \sum_{j=1}^N \partial_{x_j} p_j(x, y, u)$  the divergence of the vector  $p$ . Then, the previous equation gives in strong form for all  $n$  and  $t$

$$\frac{d}{dt} \mu_n + \frac{1}{N} \sum_{m=1}^N \partial_1 p(\xi_n, \xi_m, u)^T \mu_n + \frac{1}{N} \sum_{m=1}^N \partial_2 p(\xi_m, \xi_n, u)^T \mu_m + \nabla_\xi \phi(\xi_n, u) = 0, \quad \mu_n(T) = 0. \tag{2.4}$$

Additionally, the first-order optimality conditions contain the state equation

$$-\frac{d}{dt} \xi_n + \frac{1}{N} \sum_{m=1}^N p(\xi_n, \xi_m, u) = 0, \quad \xi_n(0) = \xi_n^I, \tag{2.5}$$

and the optimality condition. The control is then determined by

$$\frac{1}{N^2} \sum_{m=1}^N \sum_{n=1}^N \mu_n^T \partial_u p(\xi_n, \xi_m, u) + \frac{1}{N} \sum_{n=1}^N \nabla_u \phi(\xi_n, u) = 0, \quad \forall t \tag{2.6}$$

Under suitable assumptions on the second derivatives  $\nabla_{uu}^2 \phi$  and  $\nabla_{uu}^2 p(\xi_n, \xi_m, u)$  the control  $u$  can be expressed explicitly in terms of  $\vec{\mu}$  and  $\vec{\xi}$ . e.g., in the case  $p$  independent of  $u$  the strict convexity of  $\phi$  is sufficient. For a formal proof and the corresponding statement we refer to the literature, e.g. to [18]. As therein, we therefore remove  $u$  from the previous conditions. Hence, we study the meanfield equations for (2.5) and (2.4) only and, for simplicity of notation, keep  $u$  as a variable. This variable  $u$  is expressed in terms of  $\vec{\xi}$  and  $\vec{\mu}$ , respectively, as given by Equation (2.6).

In Section (2.2) we will derive the evolution equation for the joint  $2N$  body density for the states  $\xi_n, \mu_n, n = 1, \dots, N$ , i.e. the corresponding probability density. Then, in Section (2.3) we will carry out a mean field limit under the assumption of identical and independently distributed particles to arrive at effective one agent equations for the states and the Lagrange multipliers.

**2.2. The N-agent density of the optimality conditions.** Here, we derive the general relation between the solution of a system of ordinary differential equations and the (degenerate) probability density, concentrated on discrete values, of its solution. We first present a general result for a state  $\eta_n \in \mathbb{R}^K$  and  $n = 1, \dots, N$ . Later, we apply the result to the specific system Equation (2.1). In general, the following result holds true.

PROPOSITION 2.1. *Assume  $n = 1, \dots, N$  agents behave according to the following system of ordinary differential equations:*

$$\partial_t \eta_n = v_n(\vec{\eta}), \quad n = 1, \dots, N.$$

We assume each state of agent  $n$   $\eta_n \in \mathbb{R}^K$  and an initial datum  $\eta_n(0) = \eta_0^I$  be given. Also, we assume that the velocity  $v_n: \mathbb{R}^K \rightarrow \mathbb{R}^K$  of the agent  $n$  is a known function.

Defining a measure  $F(\cdot, t)$  on  $\mathbb{R}^{KN}$  as  $F(\vec{y}, t) = \prod_{n=1}^N \delta(y_n - \eta_n(t))$ , then  $F$  satisfies in the weak sense

$$\partial_t F(\vec{y}, t) + \sum_{n=1}^N \operatorname{div}_{y_n} (v_n(\vec{y}) F(\vec{y}, t)) = 0$$

and  $F(\vec{y}, 0) = \prod_{n=1}^N \delta(y_n - \eta_0^I)$ .

*Proof.* Let  $\psi$  be an arbitrary, compactly supported smooth function on  $\mathbb{R}^K$ . A formal computation shows that

$$\partial_t F(\vec{y}, t) = - \sum_{n=1}^N v_n(\vec{\eta})^T \nabla \delta(y_n - \eta_n) \prod_{k \neq n, k=1}^N \delta(y_k - \eta_k(t))$$

and therefore in the weak form we obtain the assertion by integration on  $\mathbb{R}^K$

$$\begin{aligned} \int \psi(\vec{y}) \partial_t F(\vec{y}, t) \, d\vec{y} &= \int \sum_{n=1}^N v_n(\vec{y})^T \nabla_{y_n} \psi(\vec{y}) \prod_{k=1}^N \delta(y_k - \eta_k(t)) \, d\vec{y} \\ &= \int \sum_{n=1}^N v_n(\vec{y})^T \nabla_{y_n} \psi(\vec{y}) F(\vec{y}, t) \, d\vec{y}. \end{aligned}$$

Integration by parts gives the strong form as

$$\partial_t F(\vec{y}, t) + \sum_{n=1}^N \operatorname{div}_{y_n} (v_n(\vec{y}) F(\vec{y}, t)) = 0.$$

□

The previous proposition is applied to the particle model (2.1). We set  $\vec{\eta} = (\vec{\xi}, \vec{\mu})$  and  $\vec{y} = (\vec{x}, \vec{z})$  in Equation (2.4) and (2.5) to obtain

$$\partial_t F(\vec{x}, \vec{z}, t) + \frac{1}{N} \sum_{m=1}^N \sum_{n=1}^N \operatorname{div}_{x_n} [F(\vec{x}, \vec{z}, t) p(x_n, x_m, u)] \tag{2.7a}$$

$$- \frac{1}{N} \sum_{n=1}^N \sum_{m=1}^N \operatorname{div}_{z_n} [F(\vec{x}, \vec{z}, t) \partial_1 p(x_n, x_m, u)^T z_n] \tag{2.7b}$$

$$- \frac{1}{N} \sum_{n=1}^N \sum_{m=1}^N \operatorname{div}_{z_n} [F(\vec{x}, \vec{z}, t) \partial_2 p(x_m, x_n, u)^T z_m] \tag{2.7c}$$

$$-\sum_{n=1}^N \operatorname{div}_{z_n} [F(\vec{x}, \vec{z}, t) \nabla_x \phi(x_n, u)] = 0, \tag{2.7d}$$

where again  $\partial_1 p$  and  $\partial_2 p$  denote the corresponding  $K \times K$  Jacobi matrices of  $p$ .

**2.3. Derivation of the meanfield limit for the single agent density.** Equation (2.7) is posed on a higher-dimensional space  $\mathbb{R}^{2KN+1}$  and therefore we apply an IID ansatz in Equation (2.7). Hence, we **assume** that the  $2N$ -particle density fulfills

$$F(\vec{x}, \vec{z}, t) = \prod_{n=1}^N f(x_n, z_n, t) \tag{2.8}$$

for  $f: \mathbb{R}^K \times \mathbb{R}^K \times \mathbb{R}_+ \rightarrow \mathbb{R}$  with  $f \in \mathcal{M}_0 := \{f: \int_{\mathbb{R}^K \times \mathbb{R}^K} f \, dx dz = 1\}$ , that is the manifold of probability densities. The assumption (2.8) is common in the derivation of mean-field equations, see e.g. [14], and it relies on the observation that in many particle systems the individual particles are identical and independent. Therefore, we may assume that the probability density  $F$  is in fact a product of single particle distributions  $f$ .

In order to obtain the corresponding equation for  $f$  we integrate the equation for  $F$  on  $d\vec{x}_- \, d\vec{z}_-$  where  $\vec{x}_- = (x_2, \dots, x_N)$  and  $\vec{z}_- = (z_2, \dots, z_N)$ . This approach is as in the derivation of the BBGKY hierarchy and we refer e.g. to [13, 14] for more details. The following derivation is not rigorous in the sense that more assumptions on the agent dynamics are required to rigorously prove a decomposition of the kinetic density in single particle distributions (2.8). An example of suitable assumptions and the corresponding derivation of the resulting equation is given in [9]. In the following, we present a formal computation using Equation (2.8) as assumption.

$$\partial_t f(x_1, z_1, t) + \frac{1}{N} \sum_{m=1}^N \operatorname{div}_{x_1} \left[ \int F(\vec{x}, \vec{z}, t) p(x_1, x_m) \, d\vec{x}_- \, d\vec{z}_- \right] \tag{2.9a}$$

$$- \frac{1}{N} \sum_{m=1}^N \operatorname{div}_{z_1} \left[ \int F(\vec{x}, \vec{z}, t) \partial_1 p(x_1, x_m, u)^T z_1 \, d\vec{x}_- \, d\vec{z}_- \right] \tag{2.9b}$$

$$- \frac{1}{N} \sum_{m=1}^N \operatorname{div}_{z_1} \left[ \int F(\vec{x}, \vec{z}, t) \partial_2 p(x_m, x_1, u)^T z_m \, d\vec{x}_- \, d\vec{z}_- \right] \tag{2.9c}$$

$$- \operatorname{div}_{z_1} \left[ \int F(\vec{x}, \vec{z}, t) \nabla_x \phi(x_1, u) \, d\vec{x}_- \, d\vec{z}_- \right] = 0. \tag{2.9d}$$

From Equation (2.8) we have

$$F(x, z, t) = f(x_1, z_1, t) F_-(\vec{x}_-, \vec{z}_-, t)$$

and  $F_-(\vec{x}_-, \vec{z}_-, t) = \prod_{n=2}^N f(x_n, z_n, t)$ . This leads to the following equation for  $f(x_1, z_1, t)$

$$\begin{aligned} \partial_t f(x_1, z_1, t) + \frac{1}{N} \sum_{m=1}^N \operatorname{div}_{x_1} [f(x_1, z_1, t) \int F_-(\vec{x}_-, \vec{z}_-, t) p(x_1, x_m)] \, d\vec{x}_- \, d\vec{z}_- \\ - \frac{1}{N} \sum_{m=1}^N \operatorname{div}_{z_1} [f(x_1, z_1, t) \int F_-(\vec{x}_-, \vec{z}_-, t) \partial_1 p(x_1, x_m, u)^T z_1 \, d\vec{x}_- \, d\vec{z}_-] \\ - \frac{1}{N} \sum_{m=1}^N \operatorname{div}_{z_1} [f(x_1, z_1, t) \int F_-(\vec{x}_-, \vec{z}_-, t) \partial_2 p(x_m, x_1, u)^T z_m \, d\vec{x}_- \, d\vec{z}_-] \end{aligned}$$

$$- \operatorname{div}_{z_1} [f(x_1, z_1, t) \nabla_x \phi(x_1, u) \int F_-(\vec{x}_-, \vec{z}_-, t) d\vec{x}_- d\vec{z}_-] = 0.$$

An elementary but tedious computation leads to a closed form for  $f(x_1, z_1, t)$  upon integration with respect to  $d\vec{x}_- d\vec{z}_-$ .

$$\begin{aligned} & \partial_t f(x_1, z_1, t) + \frac{N-1}{N} \operatorname{div}_{x_1} [f(x_1, z_1, t) \int f(x_2, z_2, t) p(x_1, x_2, u)] dx_2 dz_2 \\ & - \frac{N-1}{N} \operatorname{div}_{z_1} [f(x_1, z_1, t) \int f(x_2, z_2, t) \partial_1 p(x_1, x_2, u)^T z_1 dx_2, z_2] \\ & - \frac{N-1}{N} \operatorname{div}_{z_1} [f(x_1, z_1, t) \int f(x_2, z_2, t) \partial_2 p(x_2, x_1, u)^T z_2 dx_2 dz_2] \\ & - \operatorname{div}_{z_1} [f(x_1, z_1, t) \nabla_x \phi(x_1, u)] = 0. \end{aligned}$$

In the previous equation we may take the limit for infinitely many agents  $N \rightarrow \infty$  to obtain

$$\partial_t f(x_1, z_1, t) + \operatorname{div}_{x_1} [f(x_1, z_1, t) \int f(x_2, z_2, t) p(x_1, x_2, u)] dx_2 dz_2 \tag{2.10a}$$

$$- \operatorname{div}_{z_1} [f(x_1, z_1, t) \int f(x_2, z_2, t) \partial_1 p(x_1, x_2, u)^T z_1 dx_2, z_2] \tag{2.10b}$$

$$- \operatorname{div}_{z_1} [f(x_1, z_1, t) \int f(x_2, z_2, t) \partial_2 p(x_2, x_1, u)^T z_2 dx_2 dz_2] \tag{2.10c}$$

$$- \operatorname{div}_{z_1} [f(x_1, z_1, t) \nabla_x \phi(x_1, u)] = 0. \tag{2.10d}$$

The density  $f(x_1, z_1, t)$  in Equation (2.10) still depends on the variables  $x_1, z_1$ , corresponding to the state  $x_1$  of the system and the Lagrange multiplier  $z_1$ , respectively. However, Equation (2.10) can be closed **exactly**. In order to do so, we write  $f$  in terms of the conditional probability  $f_c$  with respect to  $z_1$ . Hence, we define the conditional probability  $f_c$  as follows:

$$f_0(x_1, t) = \int f(x_1, z_1, t) dz_1, \quad f(x_1, z_1, t) = f_c(z_1 | x_1, t) f_0(x_1, t). \tag{2.11}$$

This implies that, for all  $x_1$ ,  $\int f_c(z_1 | x_1, t) dz_1 = 1$  holds. The vector-valued conditional expectation  $\mu(x_1, t) \in \mathbb{R}^K$  is then given by

$$\mu(x_1, t) = \mathbb{E}_{f_c}(x_1, t) = \int z_1 f_c(z_1 | x_1, t) dz_1 .$$

With a slight abuse of notation, we use the same symbol  $\mu$  for the conditional expectation as for the discrete Lagrange multiplier in Section 2.1. The reason for this is, that we will show in Section 4 a certain equivalence of the systems obtained in Sections 2.1 and 2.2.

This allows to simplify Equation (2.10). With the definitions, Equation (2.10) is closed in terms of  $f_0$  and the  $K$ - vector  $\mu$ . We summarize the findings in the following proposition.

**PROPOSITION 2.2.** *Assume  $f$  and  $u$  as in (2.10) and  $f_0$  and  $\mu$ , given by Equation (2.11). Then,  $f_0, \mu$  satisfy*

$$\partial_t f_0(x_1, t) + \operatorname{div}_{x_1} [f_0(x_1, t) G_f(x_1, t)] = 0, \tag{2.12a}$$

$$f_0(x_1, 0) = f^I(x_1) \tag{2.12b}$$

$$\partial_t[\mu(x_1, t)f_0(x_1, t)] + \operatorname{div}_{x_1}[f_0(x_1, t)G_f(x_1, t)\mu(x_1, t)^T] \tag{2.12c}$$

$$+ f_0(x_1, t)\partial_x G_f(x_1, t)^T \mu(x_1) + f_0(x_1)b_{f\mu}(x_1, t) + f_0(x_1)\nabla_x \phi(x_1, u) = 0, \tag{2.12d}$$

$$\mu(x_1, T) = 0, \tag{2.12e}$$

with the  $K$ - vectors  $G_f, b_{f\mu}$  given by

$$G_f(x_1, t) = \int f_0(x_2, t)p(x_1, x_2, u(t)) \, dx_2, \tag{2.13a}$$

$$b_{f\mu}(x_1, t) = \int f_0(x_2, t)\partial_2 p(x_2, x_1, u(t))^T \mu(x_2, t) \, dx_2, \tag{2.13b}$$

and the  $K \times K$  Jacobian given by

$$\partial_x G_f(x_1, t) = \int f_0(x_2, t)\partial_1 p(x_1, x_2, u(t)) \, dx_2. \tag{2.14}$$

Recall, that in (2.12)(b)-(c), we use the standard definition of the  $K$ - vector valued divergence of a  $K \times K$  matrix:  $\operatorname{div}(A)_j = \sum_k \partial_k A_{kj}$ . Clearly, the  $K \times K$  matrix  $G_f \mu^T$  has the entries  $(G_f \mu^T)_{kj} = (G_f)_k \mu_j$ .

*Proof.* For notational convenience, we suppress the dependence of the variables on the time  $t$  and control  $u$ . We compute the zero order moment in  $z_1$  of (2.10), using  $\int f_c(z_1|x_1) \, dz_1 = 1, \forall x_1$ . Then, we obtain

$$\partial_t f_0(x_1) + \operatorname{div}_{x_1}[f_0(x_1) \int f_0(x_2)p(x_1, x_2, u) \, dx_2] = 0. \tag{2.15}$$

The Equation (2.15) is closed and yields (2.12)(a). Computing the first order moment in  $z_1$  in (2.10) with the  $K$ - vector  $\mu(x_1)$  the conditional expectation  $\mu(x_1) = \int z_1 f_c(z_1|x_1) \, dz_1$ , using the identity  $\int z \operatorname{div}_z g \, dz = - \int g \, dz$  gives

$$\partial_t[\mu(x_1)f_0(x_1)] + \operatorname{div}_{x_1}\left[\left(\int f_0(x_2)p(x_1, x_2, u) \, dx_2\right)\mu(x_1)^T\right] \tag{2.16a}$$

$$+ f_0(x_1)\left(\int f_0(x_2)\partial_1 p(x_1, x_2, u) \, dx_2\right)^T \mu(x_1) \tag{2.16b}$$

$$+ f_0(x_1) \int f_0(x_2)\partial_2 p(x_2, x_1, u)^T \mu(x_2) \, dx_2 + f_0(x_1)\nabla_x \phi(x_1, u) = 0. \tag{2.16c}$$

We define the the vector  $G_f \in \mathbb{R}^K$  as  $G_f(x_1) = \int f_0(x_2)p(x_1, x_2, u) \, dx_2$ . Hence, its Jacobian is  $\partial G_f(x_1) = \int f_0(x_2)\partial_1 p(x_1, x_2, u) \, dx_2 \in \mathbb{R}^{K \times K}$ . We define the  $K$ - vector  $b_{f\mu}$  as  $b_{f\mu}(x_1) = \int f_0(x_2)\partial_2 p(x_2, x_1, u)^T \mu(x_2) \, dx_2$ . This gives by (2.15)–(2.16) the closed system for the density  $f_0$  and the  $K$ - vector  $\mu$ .

$$\begin{aligned} \partial_t[\mu(x_1)f_0(x_1)] + \operatorname{div}_{x_1}[f_0(x_1)G_f(x_1)\mu(x_1)^T] + f_0(x_1)\partial G_f(x_1)^T \mu(x_1) \\ + f_0(x_1)b_{f\mu}(x_1) + f_0(x_1)\nabla \phi(x_1) = 0, \end{aligned}$$

$$\partial_t f_0(x_1) + \operatorname{div}_{x_1}[f_0(x_1)G_f(x_1)] = 0.$$

This finishes the proof. □

Equation (2.12)(b,c) will be compared to the optimization of the meanfield limit in the next section.

**3. Optimality condition based on mean-field dynamics**

In this section we consider an approach based on **first** deriving the meanfield dynamics and **then** solving a constrained optimization problem where the constraint is given by a partial differential equation. Under IID this problem results essentially in computing admissible variations with respect to the meanfield density  $f(x,t)$ . As in the previous section, the meanfield dynamics associated with Equation (2.1) and under the IID assumption is given by

$$\partial_t f(x_1,t) + \text{div}_{x_1}[f(x_1)G_{f,u}(x_1,t)] = 0, \quad f(x_1,0) = f_0^I(x_1), \tag{3.1a}$$

$$G_{f,u}(x_1,t) = \int p(x_1,x_2,u)f(x_2,t) dx_2 \tag{3.1b}$$

and initial conditions  $f_0^I$ . Further,  $u = u(t)$  is the corresponding meanfield control. The cost function (2.2) is computed on the meanfield and is given by

$$\int_0^T \int \phi(x_1,u(t))f(x_1,t)dx_1dt.$$

Hence, we study the formal constrained optimization for functions  $u(\cdot)$  by optimizing the previous functional on the manifold given by the differential Equation (3.1). The formal differential of the corresponding Lagrangian

$$\int_0^T \int \lambda(x_1,t) \left( \partial_t f(x_1,t) + \text{div}_{x_1}[f(x_1,t)G_{f,u}(x_1,t)] \right) + \phi(x_1,u)f(x_1,t)dx_1dt$$

with respect to  $f$  leads to the terminal value problem for the multiplier  $\lambda(x_1,t)$  as

$$-\partial_t \lambda(x_1,t) - \nabla_{x_1} \lambda(x_1,t)^T G_{f,u}(x_1,t) \tag{3.2a}$$

$$- \int f(x_2,t) \nabla_{x_2} \lambda(x_2,t)^T p(x_2,x_1,u) dx_2 + \phi(x_1,u) = 0 \tag{3.2b}$$

and terminal conditions

$$\lambda(x_1,T) = 0.$$

Some remarks are in order.

While the mean-field equation for the evolution of the states obviously is the same as (2.12)(a) in Section 2.3, with the obvious change in notation  $f \leftrightarrow f_0$ , the Equation (3.2) for the Lagrange multiplier seems different from Equation (2.12)(b)-(c). For one,  $\lambda$  in (3.2) is a scalar function, whereas  $\mu$  in (2.12)(b) is a  $K$ - vector. Second,  $\mu$  follows a possibly hyperbolic balance equation whereas  $\lambda$  is given by a non-conservative equation. Furthermore,  $\lambda$  is influenced through the source term by  $\phi$  whereas  $\mu$  depends on  $\nabla_x \phi(x,u)$ . Also, considering the system in dimensional units the unit of  $\lambda$  is given by the unit of  $\phi$ , i.e.,  $[\lambda] = [\phi]$ , whereas the the unit of  $\mu$  in (2.12)(b)-(c) is given by  $[\mu] = \frac{[\phi]}{[x]}$ , given the units of the functional  $\phi$  and the state space variable  $x$ .

If we consider  $f$  to be an  $L^2$ -integrable density, the previous computation is the formal Gateaux differential of the Lagrangian with respect to  $f$ . However, this does not take into account the fact that  $f$  is a probability density, i.e., the fact that  $f$  satisfies  $\int f(x,t) dx = 1, \forall t$ . So, in fact, we should consider the optimization problem for the density  $f$  rather on the manifold  $\mathcal{M} := \{f(x_1,t) : \int f(x_1,t)dx = 1, \forall t \in [0,T]\}$ . This leads to additional nonlinear constraints on  $f$  that may be handled as follows:



Equation (3.2) is derived as the strong formulation of the weak functional derivative of the Lagrangian with respect to  $f$  where we skip the dependence on  $(x_1, t)$  for notational convenience. This requires to compute variations of  $f$  in direction  $g$ . The weak formulation for any variation  $g$  of  $f$  is given by

$$\int_0^T \int \lambda \left( \partial_t g + \operatorname{div}_x [g G_{f,u} + f \partial_f G_{f,u} g] \right) + \phi(x, u) g \, dx dt = 0, \quad \forall g.$$

To compute the derivative along the tangent space of the manifold  $\mathcal{M}$ , we would have to parameterize the tangent space. The previous condition can be achieved for example by considering  $g = g(x_1, t)$  that additionally fulfills  $\int g(x_1, t) \, dx_1 = 0 \, \forall t$ .

In the case of a one dimensional state space ( $K = 1$ ), this condition can be enforced by considering variations  $g(x, t)$  such that  $g(x, t) = \partial_x \psi(x, t)$  for some sufficiently smooth  $L^1(\mathbb{R})$  function  $\psi$ . In a strong formulation, this would result in taking the gradient of Equation (3.2) and introducing the gradient of the multiplier  $\lambda$  as a new variable. In broad generality this technique has been used in [20]. Other approaches and their rigorous derivation as well as analytical results on derivatives with respect to measures are discussed in [8, 12] and briefly reviewed in the Appendix.

This trick will not work in the case of higher dimensional phase space, i.e.,  $x \in \mathbb{R}^K$ ,  $K > 1$ . However, it motivates to consider the gradient of Equation (3.2) and to introduce

$$\mu(x_1, t) = -\nabla_{x_1} \lambda(x_1, t). \tag{3.3}$$

as a new variable.  $\mu$  is now a  $K$ - vector and, in a dimensional formulation, has at least the same units as the conditional expectation  $\mu$  in Section 2.3. Formally, this leads to

$$\partial_t \mu(x_1, t) + \nabla_{x_1} [\mu^T(x_1, t) G_{f,u}(x_1, t)] \tag{3.4a}$$

$$+ \nabla_{x_1} \left[ \int f(x_2, t) \mu(x_2, t)^T p(x_2, x_1, u) \, dx_2 \right] + \nabla_{x_1} \phi(x_1, u) = 0 \tag{3.4b}$$

or, written in terms of  $G_f = G_{f,u}$  and  $b_{f\mu}(x_1, t) = \int f(x_2, t) \partial_2 p(x_2, x_1, u)^T \mu(x_2, t) \, dx_2$  as in Equation (2.13)

$$\partial_t \mu(x_1, t) + \nabla [\mu^T(x_1, t) G_f(x_1, t)] + b_{f\mu}(x_1, t) + \nabla_{x_1} \phi(x_1, u) = 0. \tag{3.5}$$

We devote the next section to a discussion of the relation between (3.5) and the derivations leading to Proposition 2.2, i.e., in particular Equation (2.12).

#### 4. Relation between the different approaches

In this section we discuss the relation between the different approaches given in Sections 2 and 3. It turns out that, the presented approaches can be linked to each other by suitable differentiation of multipliers and suitable decomposition of the kinetic densities using conditional probabilities and expectations. In the first Section 4.1 we show that, given a certain particle based semi - discretization of the system (2.12), in Section 2.3, we recover the equations for the multi -agent optimization problem (2.1-2.4). In Section 4.2 we compute that Equation (3.5), together with the equation (3.1) for the agent dynamics, is equivalent to the system (2.12) in Section 2.3.

##### 4.1. Equivalence of the multi-agent model with the mean field equations.

Here, we compare the solution of the  $N$ -agent optimization problem given by Equations (2.1)–(2.4) with the solution of the meanfield approximation in Section 2.3 given by Equation (2.10) and (2.12), respectively.

It turns out that the meanfield approximation in Section 2.3 is an exact discretization. That is, given a certain consistent discretization of the system (2.12) by a particle method, we recover the optimality Equations (2.1)–(2.4), respectively.

This result holds true for more general equations and therefore we start by discretizing a general meanfield equation similar to (2.10)

$$\partial_t f(x, z, t) = \operatorname{div}_x(A(x, t)f(x, z, t)) + \operatorname{div}_z(B(x, z, t)f(x, z, t)) \tag{4.1}$$

by a particle method in the  $x$ –direction with  $N$  particles, leaving the  $z$ –variable continuous for the moment. A particle method approximates  $f$  by  $N$  moving particles at location  $\xi_n(t)$  as

$$f(x, z, t) = \frac{1}{N} \sum_{n=1}^N \delta(x - \xi_n(t))g_n(z, t),$$

where  $g_n$  is the weight of particle  $n$ . This weight function might depend on  $z$  and  $t$ . The previous ansatz also represents a discretization of Equation (2.11) if  $g_n(z, t) = f_c(z|x_n, t)$ .

Then, we obtain for all  $z$  and any test function  $\psi(x)$  in the weak form

$$\int \psi(x)\partial_t f(x, z, t) \, dx = \frac{1}{N} \sum_{n=1}^N g_n(z, t)\nabla_x \psi(\xi_n)^T \partial_t \xi_n(t) + \psi(\xi_n)\partial_t g_n(z, t). \tag{4.2}$$

Computing the terms on the right-hand side of Equation (4.1) gives

$$\int \psi(x)\operatorname{div}_x(A(x, t)f(x, z, t)) \, dx = -\frac{1}{N} \sum_{n=1}^N g_n(z, t)\nabla_x \psi(\xi_n)^T A(\xi_n, t), \tag{4.3a}$$

$$\int \psi(x)\operatorname{div}_z(B(x, z)f(x, z, t)) \, dx = \frac{1}{N} \sum_{n=1}^N \psi(\xi_n)\operatorname{div}_z(B(\xi_n, z, t)g_n(z, t)). \tag{4.3b}$$

Comparing the  $\psi$  and the  $\nabla\psi$  terms in (4.2) and (4.3) yields the particle dynamics for  $\xi_n$  as

$$\frac{d}{dt}\xi_n(t) = -A(\xi_n, t), \quad \partial_t g_n(z, t) = \operatorname{div}_z(B(\xi_n, z, t)g_n(z, t)). \tag{4.4}$$

The Equation (4.4) is a consistent semi-discretization of the density Equation (4.1). We now relate (4.4) to the Equation (2.10) by computing the integral terms, and including the dependence on the control  $u$ :

$$A(x, t) = -\int f(x_2, z_2)p(x, x_2, u) \, dx_2 z_2 = -\frac{1}{N} \sum_{m=1}^N p(x, \xi_m, u)\rho_m(t),$$

$$B(x, z, t) = \frac{1}{N} \sum_{m=1}^N \partial_1 p(x, \xi_m, u)^T z \rho_m(t) + \frac{1}{N} \sum_{m=1}^N \partial_2 p(\xi_m, x, u)^T \mu_m(t) + \nabla_x \phi(x, u),$$

with  $\rho_m, \mu_m$  the zeroth and first order moments of the functions  $g_m$ , i.e., for each  $m$  we have  $\rho_m(t) = \int g_m(z, t) \, dz$ , and  $\mu_m(t) = \int z g_m(z, t) \, dz$ .

Computing the zeroth and first order moments of (4.4) using again the identity  $\int z \operatorname{div}_z[B(\xi_n, z, t)g_n(z, t)] \, dz = -\int B(\xi_n, z, t)g_n(z, t) \, dz$ , gives the **exact** closure equations

$$\frac{d}{dt}\xi_n(t) = \frac{1}{N} \sum_{m=1}^N p(\xi_n, \xi_m, u)\rho_m(t), \tag{4.5a}$$

$$\frac{d}{dt} \rho_n(t) = 0, \tag{4.5b}$$

$$\frac{d}{dt} \mu_n(t) = -\frac{1}{N} \sum_m \partial_1 p(\xi_n, \xi_m, u)^T \mu_n(t) \rho_m(t) \tag{4.5c}$$

$$-\frac{1}{N} \sum_m \partial_2 p(\xi_m, \xi_n, u)^T \mu_m(t) \rho_m(t) - \nabla_x \phi(\xi_n, u) \rho_n(t). \tag{4.5d}$$

Some remarks are in order.

Equation (4.4) is a consistent discretization of the Equation (2.10). Therefore, equation (4.5) is a consistent discretization of the closure system (2.12), as long as we choose a discretization method in the  $z$ -variables which allows for the identity  $\int z \operatorname{div}_z B \, dz = -\int B \, dz$  to be exact for the discretized system.

Equation (4.5) reproduces the agent based system (2.5-2.4) if  $\rho_n(t) = \int g_n(z, 0) \, dz = 1, \forall n \forall t$ . Therefore, if we start with a, uniform in  $x$ -, distribution in the Lagrange parameter  $z$  with zero first order moment, at the end time  $T$ , i.e.  $\rho_n(T) = \int g_n(z, T) \, dz = 1, \forall n$ , and  $\mu_n(T) = \int z g_n(z, T) \, dz = 0, \forall n$ , we obtain the agent based system (2.4)–(2.5) exactly. Hence, for the special case of uniform terminal conditions with zero expectation the given semi-discretization, (2.12) is equivalent to the multi agent optimization system (2.5 - 2.4).

So, the difference in the result between solving (2.10) by some other arbitrary discretization method, and solving the agent based system (2.4-2.5), is solely given by the choice of discretization methods at terminal time and the corresponding discretization error.

**4.2. Equivalence of the meanfield limit for the combined agent - Lagrange multiplier meanfield system (2.12) and the optimality system based on optimizing the meanfield dynamics(3.5).** Next, we discuss relation between Equation (2.12)(b) and Equation (3.5). Recall, that (2.12) has been obtained by the meanfield limit of the optimized discrete agent system. The adjoint variable  $\mu$  is the conditional expectation of the meanfield distribution in both primal and Lagrange variables. On the contrary, Equation (3.5) has been obtained as Gateaux derivative of the meanfield optimization problem (3.1) and then differentiation with respect to the spatial variable. Here,  $\mu(x, t) = \nabla_x \lambda(x, t)$  and  $\lambda$  is the continuous Lagrange multiplier function.

In order to compare (3.5) and Equation (2.12) we start with Equation (3.5) and use the meanfield dynamics

$$\partial_t f_0(x_1, t) + \operatorname{div}_x [f_0(x, t) G_f(x, t)] = 0$$

to obtain an equation for  $\mu f_0$ .

This leads to the equivalent Equation (4.6) as follows

$$0 = \partial_t [f_0(x_1, t) \mu(x_1, t)] + \operatorname{div}_{x_1} [f_0(x_1, t) G_f(x_1, t) \mu^T(x_1, t)] \tag{4.6a}$$

$$+ f_0(x_1, t) \partial G_f^T(x_1, t) \mu(x_1, t) \tag{4.6b}$$

$$+ f(x_1, t) [\nabla_{x_1} b_{f\mu}(x_1, t) + \nabla_x \phi(x_1, u)] + f_0(x_1, t) S(x_1, t), \tag{4.6c}$$

$$S(x_1, t) = \partial \mu^T(x_1, t) G_f(x_1, t) - (G_f^T(x_1, t) \nabla_{x_1}) \mu(x_1, t). \tag{4.6d}$$

Equation (4.6) follows from the following elementary computation where we omit the dependence on  $(x_1, t) \in \mathbb{R}^K \times \mathbb{R}$ . The  $i$ -th component of  $\mu$  fulfills

$$0 = \mu_i \partial_t f_0 + \mu_i \sum_{j=1}^K \partial_{x_j} (f_0(G_f)_j) = \mu_i \partial_t f_0 + \sum_{j=1}^K \partial_{x_j} [f_0(G_f)_j \mu_i] - \sum_{j=1}^K f_0(G_f)_j \partial_{x_j} \mu_i,$$

and hence

$$\mu \partial_t f_0 + \operatorname{div}_x [f_0 G_f \mu^T] - f_0 [G_f^T \nabla_x] \mu = 0. \tag{4.7}$$

Also, we obtain from Equation (3.4)

$$\begin{aligned} 0 &= f_0 \partial_t \mu_i + f_0 \partial_{x_i} \left[ \sum_j \mu_j (G_f)_j \right] + f_0 \partial_{x_i} b_{f\mu} + f \partial_{x_i} \phi \\ &= f_0 \partial_t \mu_i + \sum_j f_0 (G_f)_j \partial_{x_i} \mu_j + f_0 \mu_j \partial_{x_i} (G_f)_j + f_0 [\partial_{x_i} b_{f\mu} + f_0 \partial_{x_i} \phi], \end{aligned}$$

or

$$f_0 \partial_t \mu + f_0 \partial \mu^T G_f + f_0 \partial G_f^T \mu + f_0 \nabla_x b_{f\mu} + f_0 \nabla \phi = 0. \tag{4.8}$$

Adding Equation (4.7) and Equation (4.8) we obtain (4.6). Using the definition of  $\mu = \nabla \lambda$  we observe that the components of the term  $S$  are given by  $k = 1 : K$

$$S_k = \sum_{j=1}^K (\partial_{x_k} \mu_j - \partial_{x_j} \mu_k) G_{f,j} = \sum_{j=1}^K (\partial_{x_k} \partial_{x_j} \lambda - \partial_{x_j} \partial_{x_k} \lambda) G_{f,j} = 0. \tag{4.9}$$

Hence, we have established the equivalence of the meanfield system (2.12) and the optimality system based on optimizing the meanfield dynamics (3.5).

### 5. Summary

We are concerned with active particle systems that allow for some control influence. For a class of interacting particle systems we investigate optimality conditions and their corresponding meanfield limit. The novelty of this paper is to establish the link between optimization of particle systems and the optimization of the corresponding system obtained as meanfield of the particle description. The interesting connection is on the level of the Lagrange multipliers. The gradient of the multipliers of the meanfield system are equivalent to the conditional expectation of the meanfield limit of the multipliers of the particle system. Besides the theoretical result, this can be used to derive suitable numerical discretization schemes as outlined in Section 4.1.

#### Appendix. Suitable notions of differentials for optimal control problem.

Here, we summarize formal computations to motivate the links discussed in Section 4. Since the time-dependence is not important for the following computation we omit it.

We refer to [8, 12] for analytical results of derivatives with respect to measures. In the analysis of meanfield games the following notion of measure valued derivatives has been introduced, see [12, Section 2.2]. This notion could also be used to define proper optimality conditions for a Lagrangian. We recall the basic Definition [12, Definition 2.1]. Let  $T$  be some open set of  $\mathbb{R}$ . For any function  $\phi : \mathcal{M}(T) \rightarrow \mathbb{R}$  we say that  $\phi$  is of class  $C^1$  if there exists a continuous map  $\frac{\delta \phi}{\delta f} : \mathcal{M}(T) \times T \rightarrow \mathbb{R}$  such that for any  $f, f' \in \mathcal{M}(T)$  we have

$$\phi(f) - \phi(f') = \int_0^1 \int_T \frac{\delta \phi}{\delta f} ((1-s)f + sf', x) d(f - f')(x) ds.$$

The map  $\frac{\delta \phi}{\delta f}$  is defined up to an additive constant and it is assumed to be normalized by  $\int_T \frac{\delta \phi}{\delta f}(f, x) df(x) = 0$ . It is important to note that if  $\frac{\delta \phi}{\delta f}$  is also of class  $C^1$  w.r.t. to  $x$ , then the so-called *intrinsic* derivative  $D_\mu \phi : \mathcal{M}(T) \times T \rightarrow \mathbb{R}$  is defined by

$$D_\mu \phi(f, x) = D_x \left( \frac{\delta \phi}{\delta f}(f, x) \right).$$

We may illustrate this on the cost functional as

$$D_\mu \phi(f, x) = \partial_x \left( \frac{\partial \phi}{\partial f}(f, x) \right)$$

which can be computed explicitly for our example as follows: Define the functional  $J(f) := \int \phi(x)df(x)$ . Hence,

$$\begin{aligned} J(f) - J(f') &= \int \phi(x)d(f - f')dx = \int \int_0^1 \frac{\delta J}{\delta f}((1-s)f + sf', x)d(f - f')dsdx \\ \implies D_m J(f, x) &= D_x \frac{\delta J}{\delta f}(f, x) = \partial_x \phi(x). \end{aligned}$$

Computing the Gateaux differential of  $J$  in direction  $g$  and using  $g = \partial_x \psi$  we obtain  $\frac{\partial J}{\partial f}[-\psi] = -\int \phi(x)\partial_x \psi(x)dx$  for any  $\psi$  sufficiently smooth. Hence, we obtain the weak form of the intrinsic derivative. Similar computations may be carried out for the Lagrangian of the optimal control problem. We consider a functional  $J: \mathcal{M} = \mathcal{M}(\mathbb{R}) \rightarrow \mathbb{R}$  given e.g. by  $J(f) = \int \phi(x)df(x)$  as before and we compute variations of the functional in a subspace of  $\mathcal{M}$ . For any given  $f \in \mathcal{M}$  and any fixed  $\psi \in C^1(\mathbb{R}; \mathbb{R})$  we define  $\eta(s, \cdot) \in \mathcal{M}$  to be the weak solution to

$$\partial_s \eta(s, x) + \partial_x (\psi(x)\eta(s, x)) = 0, \eta(0, x) = f(x). \tag{6.1}$$

Then, we define the gradient of  $J$  at  $f$  as

$$\frac{\partial J}{\partial f}(f) := \lim_{s \rightarrow 0} \frac{J(\eta(s, \cdot)) - J(f)}{s}. \tag{6.2}$$

In case of the given example we simply obtain

$$\frac{\partial J}{\partial f}(f) = \int \phi(x)\partial_s \eta(0, x)dx = \int \phi(x)\partial_x (-\psi(x)\eta(0, x))dx = \int \partial_x \phi(x)f(x)\psi(x)dx.$$

This computation formalizes a notion of differentials in arbitrary spatial dimensions that is **not based on variations of the density function**, but based on the derivative with respect to particle paths. To this end we write the density function

$$f(x) = \int \delta(x - \xi(s)\omega(s))ds, \int \omega(s)ds = 1.$$

This implies writing the probability density  $f$  in terms of a continuum of weighted particle paths  $\eta(s)$  with some weight  $\omega$ . Using this form of  $f(x)$  obviously implies the condition  $\int f(x)dx = 1$  and therefore  $f$  being a probability density.

Taking the derivative with respect to the particle paths  $\eta(y)$  gives  $g(x) = -\int \nabla \delta(x - \eta(s))^T \delta \eta(s)\omega(s) ds$ , which immediately implies  $\int g(x) dx = 0$ . Integrating  $g$  against any function  $h(x)$  gives

$$\int h(y)g(y) dy = \int \nabla_x h(\eta(s))^T \delta \eta(s)\omega(s)ds$$

which in the one dimensional case corresponds, up to a sign, setting  $g = \partial_x \psi$ .

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