OPTIMAL CONTROL OF THE STATIONARY QUANTUM DRIFT-DIFFUSION MODEL[*]

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Abstract. In this work an optimal control problem for a stationary quantum drift diffusion (QDD) model is analyzed. This QDD model contains four space-dependent observables: The nonnegative particle density of electrons, the electrostatic potential, the quantum quasi-Fermi potential and the current density. The goal is to optimize the shape of quantum barriers in a quantum diode. Existence of optimal solutions is proved. Moreover, first-order necessary optimality conditions are derived.

Key words. Optimal control, quantum drift diffusion model, optimality conditions.

Subject classifications. 35J55, 49J20, 49K20.

1. Introduction

Ultra-small semiconductor devices exhibit electronic performances relying intrinsically on quantum-mechanical effects. In particular, in certain switching situations the electric current flowing through the device depends in a non-monotone way on the applied voltage. This important phenomenon is known as *negative differential resistance* (NDR) effect. Aside from finding tractable mathematical models for NDR effects, the question of optimizing the system's parameters with respect to desired performances has raised considerable attention in the literature; see, e.g., in [4, 6, 7, 12] for optimal control of a drift-diffusion model. Furthermore, we refer to [8], where an inverse problem for semiconductor equations was considered that arises in modelling a laser beam induced current (LBIC). For engineering aspects we refer to [15, 16, 17].

In this work we want to optimize the shape of quantum barriers in a quantum diode to achieve for a given external voltage V_D an optimal current I_d. The quantum diode consists of several sandwiched crystals of different ground energy levels whose gaps are described by the quantum barrier function B. The quantum diode's performance is overall determined by the location, the width and the ground energy values of the involved crystals. While the crystals' locations are more or less limited by technological possibilities, their length and their quality (thus, their ground energy's value) are variable. In particular, one can optimize length and quality to get as close as possible to a desired IV-curve.

It is the present paper's plan to investigate a mathematical model for this optimization procedure. The goal of the optimization is to determine amongst a class of admissible barrier functions the optimal B to achieve a desired IV-curve. We suppose the set of admissible barrier functions to be parameterized by ℓ variables ranging in the set of admissible controls U_{ad}.

The paper is organized in the following manner: In Section 2 we introduce the stationary quantum drift diffusion (QDD) model, prove existence of H^1 solutions and derive a-priori bounds. The optimal control problem is formulated in Section 3. Existence of optimal solutions is shown utilizing the a-priori bounds derived in Section 3.

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We present first-order necessary optimality conditions in Section 4.

2. The quantum drift diffusion model

The investigations concern a stationary, i.e., time-independent, unipolar QDD model constituted by a system of coupled partial differential equations. The spatial variable $\mathbf{x}$ ranges in the devices' domain W. Having in mind realistic shapes for ultra-small devices we assume W to be a cuboid in d space dimensions, $d=1,2$ or $d=3$:

$$W =]0,L_1[\times \ldots \times]0,L_d[\quad \text{with} \quad L_1,\ldots,L_d > 0. \tag{A1}$$

Typically the diode's boundary Γ splits into a contact region Γ_D and an insulating region Γ_N. It is quite realistic to assume that Γ_D consists of two opposing lateral surfaces

$$\Gamma_D = \{0,L_1\} \times [0,L_2] \times \ldots [0,L_d], \tag{A2}$$

while the insulating region is $\Gamma_N = \Gamma \setminus \Gamma_D$. Obviously, $\Gamma_N = \emptyset$ for $d=1$.

2.1. The model equations. In the framework of the stationary QDD model the diode's performance is described by four space-dependent observables: The non-negative electron's particle density n, the electrostatic potential V, the quantum quasi-Fermi potential F and the current density $\vec{J}$. The diode's parameters are the effective mass of electrons m, the temperature of the electron gas T, the positive, constant mobility of electrons μ, the positive, constant permittivity of the diode's underlying crystal ε, the time-independent, non-negative doping profile C, and the time-independent quantum barrier function $B : W \to \mathbb{R}$. The quantum barrier function B represents the ground energy's gap of one (or more) crystals with respect to a reference crystal. B vanishes in regions, where the reference crystal is present, whereas B does not vanish in a crystal whose ground energy is different from the reference crystal's ground energy. We suppose

$$B,C \in L^\infty(W). \tag{A3}$$

For the notion of Lebesgue and Sobolev spaces we refer the reader to [1], for instance.

The quantum quasi-Fermi potential F acts as the electron's velocity potential,

$$\vec{J} = \mu n \nabla F \quad \text{in } W.$$

Corresponding to the conservation of mass the current density is divergence free:

$$\nabla \cdot \vec{J} = 0 \quad \text{in } W.$$

The electrostatic potential V is self-consistent, i.e.,

$$-\epsilon \, \Delta V = q \, (n - C) \quad \text{in } W,$$

where $\epsilon \approx 11.6 \cdot 10^{-12} \frac{\text{As}}{\text{Vm}}$ is the — assumingly: constant — dielectricity constant of the underlying crystal, and the quantum quasi-Fermi potential F is

$$F = -\frac{\hbar^2}{6m} \frac{\Delta \sqrt{n}}{\sqrt{n}} + k_B T \log n + qV + B \quad \text{in } W,$$

where $\hbar \approx 6.626 \cdot 10^{-34} \text{J}s$ is Planck's constant, $k_B \approx 1.38 \cdot 10^{-23} \frac{\text{J}}{\text{K}}$ is Boltzmann's constant and $q \approx 1.6 \cdot 10^{-19} \text{As}$ is the elementary charge. The term $-\frac{\hbar^2}{6m} \frac{\Delta \sqrt{n}}{\sqrt{n}}$ is Bohm's

Quantity	s	Order of magnitude (SI units)
$\mathbf{x}$	L	$7.5 \cdot 10^{-8}$
n	$\overline{C}$	10^{24}
V	$U_{th} = k_B T/q$	$6.6 \cdot 10^{-3}$
C	$\overline{C}$	10^{24}
F	$k_B T$	10^{-21}
B	$k_B T$	10^{-21}
$\vec{J}$	$\mu \overline{C} k_B T/L$	$3.5 \cdot 10^{10}$

TABLE 2.1. *Scaling factor s for the involved quantities satisfying Quantity = s times scaled Quantity.*

quantum potential; see [2]. The effective electron mass m is typically about one tenth of the electron mass at rest $m \approx 10^{-31}$kg; see [12, 13].

It is convenient to introduce scaled variables. In Table 2.1 we give the scaling factor s for the involved quantities: Quantity $= s$ times scaled Quantity. Moreover, we use $\mu = 2.08 \frac{\mathrm{Am}^2}{J}$ and $T = 77K$. In what follows we denote the scaled variables with the same symbol as the corresponding unscaled variables. The scaled model equations read

$$\vec{J} = n \, \nabla F \qquad\qquad \text{in } W, \qquad (2.1a)$$

$$\nabla \cdot \vec{J} = 0 \qquad\qquad \text{in } W, \qquad (2.1b)$$

$$-\lambda^2 \, \Delta V = n - C \qquad\qquad \text{in } W, \qquad (2.1c)$$

$$F = -\varepsilon^2 \frac{\Delta \sqrt{n}}{\sqrt{n}} + \log(n) + V + B \qquad\qquad \text{in } W, \qquad (2.1d)$$

where

$$0 < \varepsilon^2 = \frac{\hbar^2}{6 k_B T m L^2} \approx 3 \cdot 10^{-3},$$

and via $\epsilon \approx 11.6 \cdot 10^{-12}$,

$$0 < \lambda^2 = \frac{\epsilon U_{th}}{q \overline{C} L^2} \approx 8.5 \cdot 10^{-4}.$$

It is convenient to use rather $\rho = \sqrt{n}$ than n. Equations (2.1) become

$$\vec{J} = \rho^2 \, \nabla F \qquad\qquad \text{in } W, \qquad (2.2a)$$

$$\nabla \cdot \vec{J} = 0 \qquad\qquad \text{in } W, \qquad (2.2b)$$

$$-\lambda^2 \, \Delta V = \rho^2 - C \qquad\qquad \text{in } W, \qquad (2.2c)$$

$$F = -\varepsilon^2 \frac{\Delta \rho}{\rho} + \log(\rho^2) + V + B \qquad\qquad \text{in } W. \qquad (2.2d)$$

Appropriate boundary conditions for (2.2) are obtained due to the following considerations, where $\nu : \Gamma \to \mathbb{R}^d$ is the outward normal vector:

a) We wish to optimize the current flowing through the device for a given external voltage V_D. V_D is applied along the contact region Γ_D, hence

$$V = V_D \quad \text{on } \Gamma_D.$$

b) The electron density ρ^2 along Γ_D depends on the device and on the surrounding electronic circuit. If V_D is "close to the equilibrium value", i.e., $V_D \approx 0$, it will be quite reasonable to assume ρ^2 do be "almost independent of V_D". As a consequence,

$$\rho = \rho_D \quad \text{on } \Gamma_D.$$

Possible choices for ρ_D are $\rho_D =$ "variational minimum value of an energy functional", see [11], or $\rho_D = \sqrt{C}$ leading to vanishing space charge on Γ_D; see [12].

c) In (2.2) the unknown function F can be viewed as a potential for the velocity field for electrons. Hence one has to prescribe F along the contact region Γ_D where the current enters the device.

$$F = F_D \quad \text{on } \Gamma_D.$$

In thermal equilibrium $V_D = 0$ there is no current at all which canonically leads to $F_D = 0$ (or another constant). If $V_D \neq 0$ then there will a current flow through the device and F_D has to be changed. Thus, F_D depends on V_D. A possible choice is $F_D = V_D$; see [12].

d) Along the insulating region the electric field is expected to have no component orthogonal to the device. Thus

$$\frac{\partial V}{\partial \nu} = 0 \quad \text{on } \Gamma_N.$$

e) Along the insulating region the current density $\vec{J}$ has only tangential components. As $\rho \neq 0$ can be expected we deduce via $\vec{J} = \rho^2 \nabla F$,

$$\frac{\partial F}{\partial \nu} = 0 \quad \text{on } \Gamma_N.$$

f) The quantum mechanical Bohm potential $-\varepsilon^2 \frac{\Delta \rho}{\rho}$, the diffusion potential $\log(\rho^2)$, the drift potential V and the barrier potential B all contribute to the velocity field ∇F and thus determine $\vec{J}$. Aside from the barrier potential B, one has to expect that none of these contributions has a component orthogonal to the device. Via d) and e) we deduce $\frac{\partial \log(\rho^2)}{\partial \nu} = 0$ on Γ_N. As we expect $\rho \neq 0$, we deduce

$$\frac{\partial \rho}{\partial \nu} = 0 \quad \text{on } \Gamma_N.$$

We obtain

$$-\nabla \cdot (\rho^2 \nabla F) = 0 \qquad\qquad \text{in } W, \qquad\qquad (2.3\text{a})$$

$$-\varepsilon^2 \Delta \rho = \rho \big(F - V - B - \log(\rho^2) \big) \qquad\qquad \text{in } W, \qquad\qquad (2.3\text{b})$$

$$-\lambda^2 \Delta V = \rho^2 - C \qquad\qquad \text{in } W, \qquad\qquad (2.3\text{c})$$

$$F = F_D, \ \rho = \rho_D, \ V = V_D \qquad\qquad \text{on } \Gamma_D, \qquad\qquad (2.3\text{d})$$

$$\frac{\partial F}{\partial \nu} = \frac{\partial \rho}{\partial \nu} = \frac{\partial V}{\partial \nu} = 0 \qquad\qquad \text{on } \Gamma_N. \qquad\qquad (2.3\text{e})$$

For the sake of brevity we set

$$H_b = H^1(W) \cap L^\infty(W),$$

which is a Banach space supplied with the canonical norm

$$\|\varphi\|_b = \|\varphi\|_{H^1(W)} + \|\varphi\|_{L^\infty(W)} \quad \text{for } \varphi \in H_b.$$

For $k \in \mathbb{N}$ we set

$$(H_b)^k = \underbrace{H_b \times \ldots \times H_b}_{k-\text{times}}$$

endowed with the natural product topology. Recall that in the one-dimensional case $H^1(W)$ is continuously embedded in $L^\infty(W)$ and we deduce $H_b = H^1(W) \cap L^\infty(W) = H^1(W)$. We assume henceforth

$$F_D, \rho_D, V_D \in H_b \qquad\qquad\qquad (\mathbf{A4})$$

and

$$\operatorname*{essinf}_{\mathbf{x} \in W} \rho_D(\mathbf{x}) > 0. \qquad\qquad\qquad (\mathbf{A5})$$

In (2.3) the square of the electron density $\rho = \rho(\mathbf{x}) \geq 0$, the quantum quasi-Fermi level $F = F(\mathbf{x})$, and the electric potential $V = V(\mathbf{x})$ are unknowns. The current density is given by $\vec{J} = \rho^2 \nabla F$.

Equations (2.3) possibly have several solutions. Existence of weak solutions in H^1 - shorthanded as "H^1solutions" - is established in [3, 13, 18]. H^1solutions of (2.3) belong to the Sobolev space

$$H_\circ = H_0^1(W \cup \Gamma_N) = \big\{ \varphi \in H^1(W) \, \big| \, \varphi = 0 \text{ on } \Gamma_D \big\}.$$

Since Γ_D consists of two opposing lateral surfaces the Sobolev space $H_\circ$ allows for a Poincaré inequality: there exists a constant $C_P > 0$ such that

$$\int_W \varphi^2 \, \mathrm{d}\mathbf{x} \leq C_P \int_W |\nabla \varphi|^2 \, \mathrm{d}\mathbf{x} \quad \text{for all } \varphi \in H_\circ. \qquad\qquad (2.4)$$

As a consequence, the bilinear form

$$\langle \varphi, \psi \rangle_{H_\circ} = \int_W \nabla \varphi \cdot \nabla \psi \, \mathrm{d}\mathbf{x} \quad \text{for } \varphi, \psi \in H_0^1(W)$$

is an inner product in $H_\circ$ and $(H_\circ, \langle \cdot, \cdot \rangle_{H_\circ})$ is a Hilbert space.

DEFINITION 2.1. *The triple* (F, ρ, V) *is a* H^1*solution of* (2.3) *if and only if*

1) $F - V_D, \rho - \rho_D, V - V_D \in H_\circ$; $F \in L^\infty(W)$;
2) $\rho \geq 0$ a.e. in W;
3) for all $\varphi \in H_\circ$,

$$\int_W \rho^2 \nabla F \cdot \nabla \varphi \, d\mathbf{x} = 0, \tag{2.5a}$$

$$\int_W \varepsilon^2 \nabla \rho \cdot \nabla \varphi \, d\mathbf{x} = \int_W \rho \left(F - V - B - \log(\rho^2) \right) \varphi \, d\mathbf{x}, \tag{2.5b}$$

$$\int_W \lambda^2 \nabla V \cdot \nabla \varphi \, d\mathbf{x} = \int_W (\rho^2 - C) \varphi \, d\mathbf{x}; \tag{2.5c}$$

where in (2.5b) and in the sequel

$$0 \cdot \log(0^2) = 0^2 \cdot \log(0^2) = 0.$$

REMARK 2.2. Since the space dimension d does not exceed 3 a variational formulation characterizing ρ is available: ρ is the minimizer of

$$E(\varrho) = E_{qu}(\varrho) + E_{el}(\varrho) + \int_W \varrho^2 (B - F) \, d\mathbf{x}$$

— if $d \leq 3$ we have $\forall \rho, F \in H^1(W)$: $\rho^2 F \in L^1(W)$ ensuring directional derivatives of E exist in all directions $\phi \in H^1$ such that we indeed can pass for the minimizer of E to (2.5b) — in the $H^1(W)$-weakly closed, convex set $\rho_D + H_\circ$ (see [3]), where

$$E_{qu}(\rho) = \varepsilon^2 \int_W |\nabla \rho|^2 \, d\mathbf{x} + \int_W \rho^2 \left(\log(\rho^2) - 1 \right) d\mathbf{x}$$

is the *quantum internal energy*, i.e., Bohm's interaction energy plus the classical internal energy,

$$E_{el}(\varrho) = \frac{1}{2} \int_W |\nabla V_\circ|^2 \, d\mathbf{x} + \int_W \rho^2 V^* \, d\mathbf{x},$$

is the *electrostatic energy*, where $V_\circ$ solves

$$-\lambda^2 \Delta V_\circ = \varrho^2 - C, \quad V_\circ \in H_\circ,$$

uniquely in $H_\circ$ and V^* solves

$$-\lambda^2 \Delta V^* = 0, \quad V^* - V_D \in H_\circ,$$

uniquely in $H^1(W)$, i.e., the function V^* is the Laplace-extension of the boundary data V_D.

REMARK 2.3.
   a) The functional E has at most one minimizer in $\rho_D + H_\circ$; see [11].
   b) In Definition 2.1 we require $F \in L^\infty(W)$. Due to the maximum principle one can deduce $F \in L^\infty(W)$ from (2.5a) via $F_D \in L^\infty(W)$ - *provided one has a priori estimates ensuring* $\inf_W \rho > 0$. However, available proofs of $\inf_W \rho > 0$ in turn rely on $F \in L^\infty(W)$. So by requiring $F \in L^\infty(W)$ we do not want to make things unnecessarily sophisticated here.

c) Due to available results the assumption $F^\infty(W)$ is seemingly not very restrictive: up to now is not known whether (2.3) has H^1 solutions $F \notin L^\infty(W)$.

d) With the same notations as in Definition 2.1-4) the function $V = V_\circ + V^*$ is the unique $H^1(W)$-weak solution of

$$-\lambda^2 \Delta V = \rho^2 - C, \quad V - V_D \in H_\circ.$$

Furthermore, for each triple $(C, F, B) \in (L^\infty(W))^3$ and each ρ minimizing E in $\rho_D + H_\circ$, the pair (ρ, V) satisfies (2.5b), (2.5c).

e) Concerning the electrostatic energy we deduce via Poincaré's inequality

$$\frac{1}{2} \int_W |\nabla V_\circ(\rho^2 - C)|^2 \, d\mathbf{x}$$
$$\leq \frac{C_P \operatorname{meas}(W)}{2\lambda^4} \left(\|\rho\|_{L^\infty(W)}^2 + \|C\|_{L^\infty(W)} \right)^2 \quad \text{for all } \rho \in L^\infty(W),$$

where here and in the sequel "meas" is the Lebesgue measure.

Now we establish the existence of a H^1 solution and a-priori estimates. The proof can be found in the appendix.

THEOREM 2.4. *Let* (**A1**)-(**A5**) *and*

$$\varepsilon, \lambda > 0 \tag{A6}$$

hold. Then (2.3) has a H^1 solution and there is a constant $C > 0$ depending on W, ε, λ, $\|\rho_D\|_b$, $\|V_D\|_b$, $\|C\|_{L^\infty(W)}$, $\|F_D\|_b$, such that for each H^1 solution (F, ρ, V),

$$\|F\|_b + \|\rho\|_b + \|V\|_b \leq C e^{C e^{\|B\|_{L^\infty(W)}}}. \tag{2.6}$$

2.2. The current. The Dirichlet boundary Γ_D splits into two (disjoint) parts

$$\Gamma_D^1 = \{0\} \times W_D \quad \text{and} \quad \Gamma_D^2 = \{L_1\} \times W_D$$

with $W_D =]0, L_2[\times \ldots \times]0, L_d[$. The current $I_i(F, \rho)$ flowing through Γ_D^i, $i = 1$ or $i = 2$, is given by

$$I_i(F, \rho) = (-1)^i q \int_{W_D} (\vec{J} \cdot \vec{e}_1)(z_i, x_2, \ldots, x_d) \, d(x_2, \ldots, x_d)$$

$$= (-1)^i q \int_{W_D} (\rho^2 \nabla F \cdot \vec{e}_1)(z_i, x_2, \ldots, x_d) \, d(x_2, \ldots, x_d), \tag{2.7}$$

where $z_1 = 0$, $z_2 = L_1$ and $\vec{e}_1 = (1, 0, \ldots, 0)^T$. We set

$$I(F, \rho) = I_1(F, \rho).$$

In (2.7) we have to evaluate the gradient ∇F along Γ_D which will not be possible for any F in $H^1(W)$. This technical difficulty can easily be handled by using an alternative formula for $I(F, \rho)$:

- If $d=1$ then $W=]0,L_1[$ and the current density $J=\vec{J}$ will be constant. Thus,

$$I(F,\rho)=-\frac{q}{L_1}\int_0^{L_1}J\cdot 1\,\mathrm{d}\mathbf{x}\quad\text{for }d=1.\tag{2.8}$$

- For $d>1$ then we introduce for arbitrary $l\in]0,L_1[$ the cuboid

$$W_l=]0,l[\times]0,L_2[\times\ldots\times]0,L_d[\subset W.$$

Recall that $\vec{J}$ is divergence-free and that there is no current-flow across the Neumann-boundary. Therefore, we obtain for $l\in]0,L_1[$

$$\begin{aligned}0&=\int_{W_l}\nabla\cdot\vec{J}\mathrm{d}\mathbf{x}=\int_{\partial W_l}\vec{J}\cdot\nu\,\mathrm{d}\mathbf{s}\\&=-\int_{\Gamma_D^1}\vec{J}\cdot\vec{e}_1\,\mathrm{d}\mathbf{s}+\int_{\Gamma_D^2}\vec{J}\cdot\vec{e}_1\,\mathrm{d}\mathbf{s}+\int_{\Gamma_N\cap\partial W_l}\vec{J}\cdot\nu\,\mathrm{d}\mathbf{s}\\&=\int_{W_D}\Big((\vec{J}\cdot\vec{e}_1)(l,x_2,\ldots,x_d)-(\vec{J}\cdot\vec{e}_1)(0,x_2,\ldots,x_d)\Big)\mathrm{d}(x_2,\ldots,x_d).\end{aligned}$$

Consequently, we deduce from (2.7)

$$\begin{aligned}I(F,\rho)=I_1(F,\rho)&=(-1)q\int_{W_D}\big(\vec{J}\cdot\vec{e}_1\big)(0,x_2,\ldots,x_d)\mathrm{d}(x_2,\ldots,x_d)\\&=-q\int_{W_D}\big(\vec{J}\cdot\vec{e}_1\big)(l,x_2,\ldots,x_d)\mathrm{d}(x_2,\ldots,x_d)\quad\text{for }l\in]0,L_1[,\end{aligned}$$

such that via integration from $l=0$ to $l=L_1$,

$$I(F,\rho)=-\frac{q}{L_1}\int_W\vec{J}\cdot\vec{e}_1\,\mathrm{d}\mathbf{x}=-\frac{q}{L_1}\int_W\rho^2\nabla F\cdot\vec{e}_1\,\mathrm{d}\mathbf{x}\quad\text{for }d\in\{2,3\}.\tag{2.9}$$

In the sequel we use formulae (2.8) and (2.9) as definitions of $I(F,\rho)$, see Section 3.

3. The optimal control problem

In this section we introduce the optimal control problem to determine amongst a class of admissible barrier functions the optimal B to achieve a desired IV-curve. Further, we prove existence of optimal solutions.

We suppose the set of admissible barrier functions to be parametrized by ℓ, $\ell\in\mathbb{N}^*$, variables. U_{ad} is the set of admissible controls. We assume:

$$\begin{cases}\text{The set }U_{\mathrm{ad}},\ \emptyset\neq U_{\mathrm{ad}}\subseteq\mathbb{R}^\ell\text{ of control parameters is}\\\text{compact. The mapping}\\\qquad B:W\times U_{\mathrm{ad}}\to\mathbb{R}\\\text{is bounded and for all }x\in W\text{ the partial function}\\B(\mathbf{x};\cdot)\text{ is in }C^{(2,1)}(U_{\mathrm{ad}}).\text{ The set of all partial functions}\\\qquad\mathcal{B}_{\mathrm{ad}}=\{B(\cdot;u_1,\ldots,u_\ell):(u_1,\ldots,u_\ell)\in U_{\mathrm{ad}}\}\\\text{is the set of admissible barrier functions.}\end{cases}\tag{A7}$$

The gradient $\nabla_u B(\cdot;u)$ is a row vector with ℓ components. Let us present an example for the set U_{ad} and $\mathcal{B}_{\mathrm{ad}}$.

EXAMPLE 3.1. Let $\phi:\mathbb{R}^d\times]0,\infty[\to[0,\infty[$ be a function in $C_c^\infty(\mathbb{R}^d\times]0,1/10[)$ such that for all $\epsilon\in]0,1/10[$ the function $\phi(\cdot,\epsilon)$ is supported in $]-1,1[\times\mathbb{R}^{d-1}$. ϕ may be generated via mollifying a step function, where ϵ is a mollifying parameter. We obtain $\Phi:]-1,1[\times W_D\times]0,\infty[\to\mathbb{R}$ by restricting ϕ to $]-1,1[\times W_D\times]0,\infty[$. Then we choose $\theta_1,\ldots,\theta_m\in]0,L_1[$ with $0<\theta_1<\ldots<\theta_m<L_1$ and we set $\delta:=\min\{\theta_j-\theta_{j-1}:2\le j\le m\}$ for $m\in\mathbb{N}$. Putting, e.g.,

$$U_{\mathrm{ad}}=[a,A]^m\times[\delta/10,9\delta/10]^m\times[1/100,1/20]$$

for some $a,A\in\mathbb{R}$ with $0\le a<A$ and defining $B:W\times U_{\mathrm{ad}}\to\mathbb{R}$ by

$$B(x;\alpha_1,\ldots,\alpha_m,\xi_1,\ldots,\xi_m,\epsilon)=\sum_{j=1}^m\alpha_j\Phi\Big(\frac{x_1-\theta_j}{\xi_j},x_2,\ldots,x_d,\epsilon\Big),$$

we obtain a function B meeting the requirements of (**A7**) with $\ell=1+2m$. Obviously each B is the sum of re-scaled, shifted, compactly supported test functions whose supports do not intersect. $\diamond$

For control parameters $u\in U_{\mathrm{ad}}$ the quantum barrier function is $B(\cdot;u)$ and the state variables F, ρ, and V are H^1solutions of the scaled QDD model (2.3) which has, according to Theorem 2.4, for given $B(\cdot;u)$ at least one H^1solution.

We proceed by introducing the cost functional $J:H_b\times H_b\times\mathbb{R}^\ell\to[0,\infty)$ by

$$J(F,\rho,u)=\frac{1}{2}\,|I(F,\rho)-I_d|^2+\sum_{i=1}^\ell\frac{\beta_i}{2}\,|u_i|^2,$$

where the current functional is

$$I(F,\rho)=-\frac{q}{L_1}\int_W\rho^2\nabla F\cdot\vec{e}_1\,\mathrm{d}\mathbf{x},$$

$I_d\in\mathbb{R}$ is a given desired current, and the β_i's are positive regularization scalars.

LEMMA 3.2.   *The current functional $I:H_b\times H_b\to\mathbb{R}$ is twice continuously Fréchet-differentiable and its second Fréchet derivative is Lipschitz-continuous.*

A proof of Lemma 3.2 is given in the appendix.

LEMMA 3.3. *The cost functional J is weakly (lower semi-)continuous. Moreover, J is twice continuously Fréchet-differentiable and its second Fréchet derivative is Lipschitz-continuous.*

Proof. First we show that the cost J is weakly continuous. For this purpose let $\{(F^n,\rho^n,u^n)\}_{n\in\mathbb{N}}$ be a sequence in $H_b\times H_b\times\mathbb{R}^\ell$ with

$$(F^n,\rho^n,u^n)\rightharpoonup(F^*,\rho^*,u^*)\text{ in }H_b\times H_b\times\mathbb{R}^\ell\text{ as }n\to\infty.$$

Since $H^1(W)$ is compactly embedded in $L^4(W)$ for $d\le3$ (see [1]), we have

$$\left(\rho^n\right)^2\to\left(\rho^*\right)^2\text{ in }L^2(W)\text{ as }n\to\infty.$$

Moreover, $\nabla F^n\rightharpoonup\nabla F^*$ in $L^2(W;\mathbb{R}^d)$ as $n\to\infty$ which implies

$$\lim_{n\to\infty}-\frac{q}{L_1}\int_W\left(\left(\rho^n\right)^2\nabla F^n-\left(\rho^*\right)^2\nabla F^*\right)\cdot\vec{e}_1\,\mathrm{d}\mathbf{x}=0.$$

Consequently,

$$\lim_{n\to\infty}\big|I(F^n,\rho^n)-I_d\big|^2=\big|I(F^*,\rho^*)-I_d\big|^2. \tag{3.1}$$

Since $u^n\to u^*$ in $\mathbb{R}^\ell$ we directly infer that

$$\lim_{n\to\infty}|u_i^n|^2=|u_i^*|\quad\text{for }1\le i\le\ell. \tag{3.2}$$

From (3.1) and (3.2) it follows that J is weakly continuous and consequently weakly lower semi-continuous as well.

Due to Lemma 3.2 the operator I is twice continuously Fréchet-differentiable. Consequently, J is twice continuously Fréchet-differentiable at any $(\bar{F},\bar{\rho},\bar{u})\in H_b\times H_b\times\mathbb{R}^\ell$. For directions $(F,\rho,u),(\tilde{F},\tilde{\rho},\tilde{u})\in H_b\times H_b\times\mathbb{R}^\ell$ the first and second derivatives are

$$\nabla J(\bar{F},\bar{\rho},\bar{u})(F,\rho,u)=\big(I(\bar{F},\bar{\rho})-I_d\big)\nabla I(\bar{F},\bar{\rho})(F,\rho)+\sum_{i=1}^\ell\beta_i\bar{u}_iu_i \tag{3.3}$$

and

$$\begin{aligned}
&\nabla^2 J(\bar{F},\bar{\rho},\bar{u})\big((\tilde{F},\tilde{\rho},\tilde{u}),(F,\rho,u)\big)\\
&=\nabla I(\bar{F},\bar{\rho})(F,\rho)\nabla I(\bar{F},\bar{\rho})(\tilde{F},\tilde{\rho})+\sum_{i=1}^\ell\beta_i\tilde{u}_iu_i\\
&\quad+\big(I(\bar{F},\bar{\rho})-I_d\big)\nabla^2 I(\bar{F},\bar{\rho})\big((\tilde{F},\tilde{\rho}),(F,\rho)\big),
\end{aligned} \tag{3.4}$$

where ∇I and $\nabla^2 I$ are given by formulas (A.8) and (A.9) in the appendix, respectively. Since the mapping $(\bar{F},\bar{\rho})\mapsto\nabla^2 I(\bar{F},\bar{\rho})$ is Lipschitz-continuous, we conclude that $(\bar{F},\bar{\rho},\bar{u})\mapsto\nabla^2 J(\bar{F},\bar{\rho},\bar{u})$ is Lipschitz-continuous as well. □

REMARK 3.4. Advanced numerical optimization methods — like sequential quadratic programming (SQP) techniques — are known to have second-order rate of convergence properties provided the cost functional and the constraints are twice continuously Fréchet-differentiable with at least locally Lipschitz-continuous second derivatives. Due to Lemma 3.3 the cost functional has these smoothness properties. The smoothness properties of the constraints will be addressed in Lemma 4.1.

To deal with the QDD model in an abstract form, let us define the closed subset X_{ad} of the Banach space $X=(H_b)^3\times\mathbb{R}^\ell$ and the Hilbert space Y as follows

$$X_{\mathrm{ad}}=(H_b)^3\times U_{\mathrm{ad}}\quad Y=(H_\circ)^3\times\big(H^{1/2}(\Gamma_D)'\big)^3,$$

endowed with their natural product topology. Recall that $H_\circ=H_0^1(W\cup\Gamma_N)$. We identify the dual Y' of Y with

$$(H_\circ')^3\times\big(H^{1/2}(\Gamma_D)\big)^3.$$

Next we introduce the non-linear operator

$$e=(e^1,e^2,e^3,e^4,e^5,e^6):X\to Y'$$

via

$$\langle e^1(x),\varphi\rangle_{H'_\circ,H_\circ} = \int_\Omega \rho^2 \nabla F \cdot \nabla \varphi \, \mathrm{d}\mathbf{x},$$

$$\langle e^2(x),\varphi\rangle_{H'_\circ,H_\circ} = \int_W \varepsilon^2 \nabla \rho \cdot \nabla \varphi + \rho\big(V + B(\cdot;u) + \log(\rho^2) - F\big)\varphi \, \mathrm{d}\mathbf{x},$$

$$\langle e^3(x),\varphi\rangle_{H'_\circ,H_\circ} = \int_W \lambda^2 \nabla V \cdot \nabla \varphi + (C - \rho^2)\varphi \, \mathrm{d}\mathbf{x}$$

for $\varphi \in H_\circ$ and

$$e^4(x) = \tau_D(F - F_D), \quad e^5(x) = \tau_D(\rho - \rho_D), \quad e^6(x) = \tau_D(V - V_D),$$

where $x = (F,\rho,V,u) \in X$, $B = B(\cdot;u)$ and

$$\tau_D : H^1(\Omega) \to H^{1/2}(\Gamma_D)$$

is the canonical (continuous, surjective) projection from $H^1(\Omega)$ onto $H^{1/2}(\Gamma_D)$.

REMARK 3.5. One can also work on the affine space $x_D + X$ with the element $x_D = (F_D, \varrho_D, V_D, 0) \in X$ and avoid the introduction of the constraints e^i, $i = 4,5,6$ without getting any different results.

The optimal control problem can be expressed in an abstract form as

$$\min J(F,\rho,u) \quad \text{s.t.} \quad x = (F,\rho,V,u) \in X_{\mathrm{ad}} \text{ and } e(x) = 0 \text{ in } Y'. \tag{P}$$

THEOREM 3.6. *Suppose* (**A1**)-(**A7**). *Then* (**P**) *has at least one global optimal solution* $x^* = (F^*, \rho^*, V^*, u^*) \in X_{\mathrm{ad}}$.

Proof. By (**A7**) we have $U_{\mathrm{ad}} \neq \emptyset$. Due to Theorem 2.4, the set

$$E = \big\{ x = (F,\rho,V,u) \in X \,\big|\, e(x) = 0 \text{ in } Y' \big\}$$

is non-empty. Due to (**A7**), there is a constant $c_1 > 0$ with $\|B(\cdot;u)\|_{L^\infty(W)} \leq c_1$ for all $u \in U_{\mathrm{ad}}$.
Suppose that for chosen $u \in U_{\mathrm{ad}}$ the triple $(F,\rho,V) \in H_b^3$ is a H^1solution of (2.3) with $B = B(\cdot;u)$. Then we infer from (2.6) that F, ρ, and V are bounded in H_b and there exists a $\zeta \geq 0$ with

$$\zeta = \inf \big\{ J(F,\rho,u) \,|\, (F,\rho,V,u) \in X_{\mathrm{ad}} \text{ satisfies (2.3) weakly} \big\}.$$

Let us consider a minimizing sequence $\{x^n\}_{n\in\mathbb{N}}$, $x^n = (F^n, \rho^n, V^n, u^n)$, in X_{ad}, i.e., $\zeta = \lim_{n\to\infty} J(F^n, \rho^n, u^n)$ holds. We define the sequence $\{B^n\}_{n\in\mathbb{N}}$ via $B^n = B(\cdot;u_n)$, $n \in \mathbb{N}$. Then x^n satisfies (2.3) for all $n \in \mathbb{N}$. Since U_{ad} is a compact subset of $\mathbb{R}^\ell$, there is $u^* \in U_{\mathrm{ad}}$ such that, eventually by passing to a subsequence but without changing notations, $u^n \to u^*$ in $\mathbb{R}^\ell$. This implies that

$$B^n \to B^* = B(\cdot;u^*) \quad \text{as } n \text{ tends to } \infty. \tag{3.5}$$

Moreover, we find from (2.6) that that

$$(F^n, \rho^n, V^n) \rightharpoonup (F^*, \rho^*, V^*) \text{ in } H^1(W)^3 \text{ as } n \to \infty \tag{3.6}$$

and $\|F^n\|_{L^\infty(W)} + \|\rho^n\|_{L^\infty(W)} + \|V^n\|_{L^\infty(W)}$ is bounded, see Theorem 2.4. Let $x^* = (F^*, \rho^*, V^*, u^*)$. Next we prove that (F^*, ρ^*, V^*) solves (2.3) weakly. Since $H^1(W)$ is compactly embedded into $L^4(W)$ for $d \leq 3$, we infer

$$\rho^n \to \rho^* \text{ in } L^4(W) \text{ as } n \to \infty, \tag{3.7}$$

which implies that

$$(\rho^n)^2 \to (\rho^*)^2 \text{ in } L^2(W) \text{ as } n \to \infty. \tag{3.8}$$

From $\nabla F^n \rightharpoonup \nabla F^*$ in $L^2(W; \mathbb{R}^d)$ as n tends to ∞ and from (3.8) we infer

$$\lim_{n \to \infty} \int_W (\rho^n)^2 \nabla F^n \cdot \nabla \varphi \, \mathrm{d}\mathbf{x} = \int_W (\rho^*)^2 \nabla F^* \cdot \nabla \varphi \, \mathrm{d}\mathbf{x} \quad \text{for all } \varphi \in H_\circ, \tag{3.9}$$

i.e., $e^1(x^*) = 0$ in $H_\circ'$. Utilizing (3.7) we deduce via the continuity of the function $\phi : [0, +\infty[\to \mathbb{R}, \ \phi(t) = t \log t$ for $t > 0$ and $\phi(0) = 0$ that

$$\lim_{n \to \infty} \log(\rho^n(\mathbf{x})^2) = \log(\rho^*(\mathbf{x})^1) \quad \text{for} \quad \mathbf{x} \in W \text{ a.e.} \tag{3.10}$$

Furthermore, $\|\rho^n\|_{L^\infty(W)}$ is bounded. Hence, there exists a constant $c_2 > 0$ such that

$$\|2\rho^n \log \rho^n\|_{L^\infty(W)} \leq c_2.$$

Applying Lebesgue's dominated convergence theorem (see, e.g. [14]) we obtain

$$\lim_{n \to \infty} \int_W 2\rho^n \log(\rho^n) \varphi \, \mathrm{d}\mathbf{x} = \int_W 2\rho^* \log(\rho^*) \varphi \, \mathrm{d}\mathbf{x} \quad \text{for all } \varphi \in H_\circ.$$

From (3.6) and (3.7) we conclude for all $\varphi \in H_\circ$,

$$\lim_{n \to \infty} \langle e^2(x^n), \varphi \rangle_{H_\circ', H_\circ} = \langle e^2(x^*), \varphi \rangle_{H_\circ', H_\circ}. \tag{3.11}$$

Again applying (3.6) and (3.7) we find that, for all $\varphi \in H_\circ$,

$$\lim_{n \to \infty} \langle e^3(x^n), \varphi \rangle_{H_\circ', H_\circ} = \langle e^3(x^*), \varphi \rangle_{H_\circ', H_\circ}. \tag{3.12}$$

Now we turn to the constraint $e^4(x^n) = 0$. By assumption, $F_D \in H_b$. Hence,

$$F^n - F_D \rightharpoonup F^* - F_D \text{ in } H_\circ \text{ as } n \to \infty.$$

Moreover, $F^n - F_D \in H_\circ$ for all $n \in \mathbb{N}$. Thus, $F^* - F_D \in H_\circ$ and

$$e^4(x^*) = \tau(F^* - F_D) = 0. \tag{3.13}$$

Analogously, we obtain

$$e^5(x^*) = e^6(x^*) = 0. \tag{3.14}$$

Summarizing, (3.9), (3.11)-(3.14) imply $e(x^*) = 0$. By Lemma 3.3 the cost functional is weakly continuous. □

4. First-order necessary optimality conditions

This section is devoted to study first-order necessary optimality conditions for (**P**). If a constrained qualification holds, there exist Lagrange multipliers satisfying a coupled dual system of three elliptic equations.

Problem (**P**) is a non-convex programming problem so that different local minima may occur. Typically a numerical method will approximates a local minimum close to its starting value. Hence, we do not restrict our investigations to global solutions of (**P**). We assume a fixed reference solution $x^* = (F^*, \rho^*, V^*, u^*)$ and investigate certain first-order optimality conditions. For that purpose we introduce the Lagrange functional $\mathcal{L} : X \times Y \to \mathbb{R}$ associated with (**P**):

$$
\begin{aligned}
\mathcal{L}(x,p) &= J(F,\rho,u) + \langle e(x), p \rangle_{Y',Y} \\
&= \frac{1}{2} \, |I(F,\rho) - I_d|^2 + \sum_{i=1}^{\ell} \frac{\beta_i}{2} \, |u_i|^2 + \int_{\Omega} \rho^2 \nabla F \cdot \nabla p_F \, \mathrm{d}\mathbf{x} \\
&\quad + \int_W \varepsilon^2 \nabla \rho \cdot \nabla p_\rho + \rho \big(V + B(\cdot\,;u) + \log(\rho^2) - F \big) p_\rho \, \mathrm{d}\mathbf{x}, \\
&\quad + \int_W \lambda^2 \nabla V \cdot \nabla p_V + (C - \rho^2) p_V \, \mathrm{d}\mathbf{x} + \langle \tau_D(F - F_D), p_{F_D} \rangle_{H^{1/2}(\Gamma_D)', H^{1/2}(\Gamma_D)} \\
&\quad + \langle \tau_D(\rho - \rho_D), p_{\rho_D} \rangle_{H^{1/2}(\Gamma_D)', H^{1/2}(\Gamma_D)} + \langle \tau_D(V - V_D), p_{V_D} \rangle_{H^{1/2}(\Gamma_D)', H^{1/2}(\Gamma_D)},
\end{aligned}
$$

where $x = (F, \rho, V, u) \in X$ and $p = (p_F, p_\rho, p_V, p_{F_D}, p_{\rho_D}, p_{V_D}) \in Y$.

Due to Lemma 3.3 the cost functional J is continuously Fréchet differentiable and its second derivative is Lipschitz-continuous in X. In the next lemma we state that the operator e is twice continuously Fréchet-differentiable. A proof is given in the appendix.

LEMMA 4.1. *For every $\bar{x} = (\bar{F}, \bar{\rho}, \bar{V}, \bar{u}) \in X$ with $\operatorname{essinf}_W \bar{\rho} > 0$ the mapping $\bar{x} \to e(\bar{x}) \in Y'$ is twice continuously Fréchet-differentiable and its second Fréchet-derivatiuve is locally Lipschitz-continuous.*

To formulate first-order necessary optimality conditions we have to ensure that the solution x^* to (**P**) is a *regular point*.

DEFINITION 4.2. *Let $\bar{x} = (\bar{F}, \bar{\rho}, \bar{V}, \bar{u})$ be a feasible point for (**P**), i.e.,*

$$
\bar{x} \in \mathcal{F}(\mathbf{P}) = \big\{ \bar{x} \in X \,\big|\, e(\bar{x}) = 0 \text{ in } Y' \text{ and } \bar{x} \in X_{\mathrm{ad}} \big\}.
$$

Then, $\bar{x}$ is called a regular point *if the linearization $\nabla e(\bar{x}) : X \to Y'$ of the operator e at $\bar{x}$ is surjective.*

Due to Lemma 4.1 the linear operator $\nabla e(\bar{x})$ is bounded provided $\operatorname{essinf}_W \bar{\rho} > 0$ is satisfied. Certainly, $\nabla e(x^*)$ will be surjective if for any given element $f = (f_F, f_\rho, f_V, f_{F_D}, f_{\rho_D}, f_{V_D}) \in Y'$ there exists a solution $x = (F, \rho, V, u) \in X$ of

$$
\nabla e(x^*) x = f \quad \text{in } Y'. \tag{4.1}
$$

The element $x \in X$ is a solution of (4.1) if and only if

$$\int_W \big((\rho^*)^2 \nabla F + 2\rho^* \rho \nabla F^*\big) \cdot \nabla\varphi \, d\mathbf{x} = \langle f_D, \varphi \rangle_{H_\circ', H_\circ}, \tag{4.2a}$$

$$\int_W \varepsilon^2 \nabla\rho \cdot \nabla\varphi + \rho\big(V^* + B^* + \log\big((\rho^*)^2\big) - F^*\big)\varphi \, d\mathbf{x}$$
$$+ \int_W \big(\rho^*(V + \nabla_u B^* u - F) + 2\rho\big)\varphi \, d\mathbf{x} = \langle f_\rho, \varphi \rangle_{H_\circ', H_\circ}, \tag{4.2b}$$

$$\int_W \lambda^2 \nabla V \cdot \nabla\varphi + 2\rho^* \rho\varphi \, d\mathbf{x} = \langle f_V, \varphi \rangle_{H_\circ', H_\circ} \tag{4.2c}$$

for all $\varphi \in H_\circ$ and

$$F = f_{F_D}, \quad \rho = f_{\rho_D}, \quad V = f_{V_D} \quad \text{in } H^{1/2}(\Gamma_D), \tag{4.2d}$$

where $B^* = B(\cdot; u^*)$ and $\nabla_u B^* = \nabla_u B(\cdot; u^*)^T$. System (4.2) is the variational formulation of the coupled linear elliptic system

$$-\nabla \cdot \big((\rho^*)^2 \nabla F + 2\rho^* \nabla F^* \rho\big) = f_D \qquad \text{in } W, \tag{4.3a}$$

$$-\varepsilon^2 \Delta\rho + \rho\big(V^* + B^* + \log\big((\rho^*)^2\big) - F^* + 2\big)$$
$$+ \rho^*\big(V + \nabla_u B^* u - F\big) = f_\rho \qquad \text{in } W, \tag{4.3b}$$

$$-\lambda^2 \Delta V + 2\rho^* \rho = f_V \qquad \text{in } W, \tag{4.3c}$$

$$F = f_{F_D} \qquad \text{on } \Gamma_D, \tag{4.3d}$$

$$\rho = f_{\rho_D} \qquad \text{on } \Gamma_D, \tag{4.3e}$$

$$V = f_{V_D} \qquad \text{on } \Gamma_D, \tag{4.3f}$$

$$\frac{\partial F}{\partial \nu} = \frac{\partial \rho}{\partial \nu} = \frac{\partial V}{\partial \nu} = 0 \qquad \text{on } \Gamma_N. \tag{4.3g}$$

Due to the lack of coercitivity it is far from obvious that, settled on grounds of the Fredholm alternative, (4.3) has a weak solution. On the other hand it is seemingly also quite difficult to verify that (4.3) has *no solution*: The universe of linear (operator) equations is certainly much larger than the set of linear (operator) equations for which the solvability question can be settled just in terms of the involved parameters. Comparing the situation with the finite-dimensional case (aside from the use of determinants which provide to the authors' knowledge no tractable concept extendable to infinite-dimensional settings): Unless rather specific information about the coefficient matrix of a linear system (positivity, self-adjointness whatsoever) are available one will not be able to say anything about the set of solutions — except, of course, that the probability that a n times n linear system with, let us say, somewhere uniformly distributed coefficients is uniquely solvable is one. So from which properties of the coefficients could we deduce unique solvability in case of "unstructuredness"? Even in the finite-dimensional case the authors have no answer to that question and we do not think things become easier in infinite dimensional settings. As a conclusion, to decide whether $\nabla e(x^*)$ is surjective or not is not in the authors' scope. Possibly, further numerical investigations may allow to gain more insight in the subject.

On the other hand, for practical purposes the existence of associated Lagrange multipliers is quite useful to obtain information on the local minimizer x^*. Since we are interested in these information let us assume

$$\nabla e(x^*) : X \to Y' \text{ is surjective.} \tag{\textbf{A8}}$$

REMARK 4.3. If $\nabla e(x^*)$ is not surjective from $X \to Y'$ but its extension on a larger space $\tilde{X}$, X densely embedded into $\tilde{X}$, possesses specific properties (weakly singular optimal control problem [9]) one can also prove existence of Lagrange multipliers.

If (**A8**) is satisfied, the point x^* is a regular point. The KKT theorem [10, Theorem 3.2] implies that there exists a unique associated Lagrange multiplier $p^* = (p_F^*, p_\rho^*, p_V^*, p_{F_D}^*, p_{\rho_D}^*, p_{V_D}^*) \in Y$ satisfying

$$\nabla_{(F,\rho,V)} e(x^*)^\star p^* = -\nabla_{(F,\rho)} J(F^*, \rho^*, u^*) \quad \text{in } (H_b')^3, \tag{4.4}$$

where $\nabla_{(F,\rho,V)} e(x^*)^\star : Y \to (H_b')^3$ is the dual operator of $\nabla_{(F,\rho,V)} e(x^*)$, i.e.,

$$\langle \nabla_{(F,\rho,V)} e(x^*)^\star p, (F,\rho,V) \rangle_{(H_b')^3, H_b} = \langle \nabla_{(F,\rho,V)} e(x^*)(F,\rho,V), p \rangle_{Y',Y}$$

for all $(F,\rho,V,p) \in (H_b)^3 \times Y$. Certainly, (4.4) and the first-order necessary optimality condition

$$\nabla_{(F,\rho,V)} \mathcal{L}(x^*, p^*) = 0 \quad \text{in } (H_b')^3$$

are equivalent.

In the following proposition we state that the Lagrange multipliers satisfy a coupled linear elliptic system.

PROPOSITION 4.4. *Let* (**A8**) *hold. The Lagrange multipliers* p_F^*, p_ρ^* *and* p_V^* *satisfy the following coupled linear system*

$$-\nabla\big((\rho^*)^2 \nabla p_F^*\big) - \rho^* p_\rho^* = -(I(F^*, \rho^*) - I_d)\nabla_F I(F^*, \rho^*) \tag{4.5a}$$

$$-\varepsilon \Delta p_\rho^* + 2\rho^* \nabla F^* \cdot \nabla p_F^* - 2\rho^* p_V^* \tag{4.5b}$$

$$+ (V^* + B^* + \log\big((\rho^*)^2\big) - F^* + 2)p_\rho^* = -(I(F^*, \rho^*) - I_d)\nabla_\rho I(F^*, \rho^*)$$

$$-\lambda^2 \Delta p_V^* + \rho^* p_\rho^* = 0 \tag{4.5c}$$

weakly in $H_\circ$, *together with homogeneous Neumann boundary conditions on* Γ_N. *Moreover,*

$$p_{F_D}^* = (\rho^*)^2 \frac{\partial p_F^*}{\partial \nu}, \quad p_{\rho_D} = \varepsilon \frac{\partial p_\rho^*}{\partial \nu}, \quad p_{V_D}^* = \lambda^2 \frac{\partial p_\rho^*}{\partial \nu} \quad \text{in } H^{1/2}(\Gamma_D)'.$$

Proof. Since $(p_F^*, p_\rho^*, p_V^*) \in (H_\circ)^3$ the functions p_F^*, p_ρ^* and p_V^* satisfy homogeneous Dirichlet boundary conditions on Γ_D. We choose an arbitrary $(F,\rho,V) \in (H_b)^3$. Recall that the gradient $\nabla_u B(\cdot; u^*)$ is a row vector. As outlined in the proof of Lemma 4.1, see appendix, we have

$$\langle \nabla_{(F,\rho,V)} e(x^*)^\star p^*, (F,\rho,V) \rangle_{(H_b')^3, (H_b)^3} = \langle \nabla_{(F,\rho,V)} e(x^*)x, p^* \rangle_{Y',Y}$$

$$= \int_W (2\rho^* \rho \nabla F^* + (\rho^*)^2 \nabla F) \cdot \nabla p_F^* \, d\mathbf{x}$$

$$+ \int_W \rho\big(V^* + B(\cdot; u^*) + \log\big((\rho^*)^2\big) - F^* + 2\big)p_\rho^* \, d\mathbf{x}$$

$$+ \int_W \varepsilon \nabla p_\rho^* \cdot \nabla \rho + \rho^*(V + \nabla_u B(\cdot; u^*)u - F)p_\rho^* \, d\mathbf{x}$$

$$+ \int_W \lambda^2 \nabla p_V^* \cdot \nabla V - 2\rho^* p_V^* \rho \, \mathrm{d}\mathbf{x}$$

$$+ \langle p_{F_D}^*, F \rangle_{H^{1/2}(\Gamma_D)', H^{1/2}(\Gamma_D)} + \langle p_{\rho_D}^*, \rho \rangle_{H^{1/2}(\Gamma_D)', H^{1/2}(\Gamma_D)}$$

$$+ \langle p_{V_D}^*, V \rangle_{H^{1/2}(\Gamma_D)', H^{1/2}(\Gamma_D)}. \tag{4.6}$$

Choosing $F \in H_0^1(W)$ and $\rho = 0$, $V = 0$, $u = 0$ we derive from (4.6), (4.4) and (3.3)

$$\langle (I_d - I(F^*, \rho^*)) \nabla_F I(F^*, \rho^*), F \rangle_{H_b', H_b}$$

$$= \int_W (\rho^*)^2 \nabla p_F^* \cdot \nabla F - \rho^* p_\rho^* F \, \mathrm{d}\mathbf{x} = \langle -\nabla \cdot ((\rho^*)^2 \nabla p_F^*) - \rho^* p_\rho^*, F \rangle_{H_b', H_b}, \tag{4.7}$$

which gives (4.5a) in $H^{-1}(W)$. Since $H_\circ$ is dense in $H_0^1(W)$, (4.7) holds in $H_\circ'$. From (4.4), (4.6), and (4.7) we infer that

$$0 = \langle (I_d - I(F^*, \rho^*)) \nabla_F I(F^*, \rho^*), F \rangle_{H_b', H_b} - \int_W (\rho^*)^2 \nabla p_F^* \cdot \nabla F - \rho^* p_\rho^* F \, \mathrm{d}\mathbf{x}$$

$$+ \langle p_{F_D}^*, F \rangle_{H^{1/2}(\Gamma_D)', H^{1/2}(\Gamma_D)}$$

$$= - \int_\Gamma (\rho^*)^2 \frac{\partial p_F^*}{\partial \nu} F \, \mathrm{d}\mathbf{s} + \langle p_{F_D}^*, F \rangle_{H^{1/2}(\Gamma_D)', H^{1/2}(\Gamma_D)}$$

for all $F \in H_b$. If we choose $F \in H_\circ$, we find that p_F^* satisfies homogeneous Neumann boundary conditions on Γ_N. On the other hand, if $F \in H_0^1(W \cup \Gamma_D)$ we obtain

$$p_{F_D}^* = (\rho^*)^2 \frac{\partial p_F^*}{\partial \nu} \quad \text{in } H^{1/2}(\Gamma_D)'.$$

Next we choose $\rho \in H_0^1(W)$ and $F = 0$, $V = 0$, $u = 0$ we derive from (4.6), (4.4) and (3.3)

$$\langle (I_d - I(F^*, \rho^*)) \nabla_\rho I(F^*, \rho^*), \rho \rangle_{H_b', H_b}$$

$$= \int_W \varepsilon \nabla p_\rho^* \cdot \nabla \rho + 2\rho^* \nabla F^* \cdot \nabla p_F^* \rho + 2p_\rho^* \rho \, \mathrm{d}\mathbf{x}$$

$$+ \int_W \left((V^* + B(\cdot; u^*) + \log((\rho^*)^2) - F^*) p_\rho^* - 2\rho^* p_V^* \right) \rho \, \mathrm{d}\mathbf{x}$$

$$= \langle -\varepsilon \Delta p_\rho^* + 2\rho^* \nabla F^* \cdot \nabla p_F^*, \rho \rangle_{H_b', H_b}$$

$$+ \langle (V^* + B(\cdot; u^*) + \log((\rho^*)^2) - F^* + 2) p_\rho^* - 2\rho^* p_V^*, \rho \rangle_{H_b', H_b}, \tag{4.8}$$

which gives (4.5b) in $H_\circ'$. Proceeding as above we find that p_ρ^* satisfies homogeneous Neumann boundary conditions on Γ_N and

$$p_{\rho_D}^* = \varepsilon \frac{\partial p_\rho^*}{\partial \nu} \quad \text{in } H^{1/2}(\Gamma_D).$$

Choosing $V \in H_0^1(W)$ and $F = 0$, $\rho = 0$, $u = 0$ we derive from (4.6), (4.4) and (3.3)

$$0 = \int_W \lambda^2 \nabla p_V^* \cdot \nabla V + \rho^* p_\rho^* V \, \mathrm{d}\mathbf{x} = \langle -\lambda^2 \Delta p_V^* + \rho^* p_\rho^*, V \rangle_{H_b', H_b}, \tag{4.9}$$

which gives (4.5c) in $H'_\circ$. As above, it follows that p^*_V satisfies homogeneous Neumann boundary conditions on Γ_N and

$$p^*_{V_D} = \lambda^2 \frac{\partial p^*_\rho}{\partial \nu} \quad \text{in } H^{1/2}(\Gamma_D)'$$

so that the proposition is proved. □

From (**A8**) we infer the variational inequality [10]

$$\nabla_u \mathcal{L}(x^*, p^*)(u - u^*) \geq 0 \quad \text{for all } u \in U_{\text{ad}}, \tag{4.10}$$

which gives

$$\left\langle D_\beta u^* + \int_W \rho^* p^*_\rho \nabla_u B(\cdot; u^*)^T \, \mathrm{d}\mathbf{x}, u - u^* \right\rangle_{\mathbb{R}^\ell} \geq 0 \quad \text{for all } u \in U_{\text{ad}},$$

where $D_\beta = \mathrm{diag}(\beta_1, \ldots, \beta_\ell) \in \mathbb{R}^{\ell \times \ell}$ is a diagonal matrix. In particular, if u^* is an interior point of U_{ad} we will obtain the implicit formula

$$u^*_i = -\frac{1}{\beta_i} \int_W \rho^* p^*_\rho \frac{\partial B}{\partial u_i}(\cdot; u^*) \, \mathrm{d}\mathbf{x} \quad \text{for } i = 1, \ldots, \ell$$

for the components of the optimal control u^*.

Appendix A.

A.1. Proof of Theorem 2.4. The proof is divided into several steps.

Step 1. Given $M \in \mathbb{R}^+$ we introduce the convex set

$$\mathsf{C}(M) = \left\{ F \in L^2(W) \,\middle|\, \|F\|_{L^\infty(W)} \leq M \right\},$$

and we define a mapping $T_M : \mathsf{C}(M) \to H^1(W)$ in three steps.

Step 1.1. Given $F \in \mathsf{C}(M)$ we denote by $\rho(F)$ the unique minimizer of

$$\rho \mapsto E(F)(\rho) = E_{qu}(\rho) + E_{el}(\rho) + E_{qupot}(\rho) - \int_W \rho^2 F \, \mathrm{d}\mathbf{x}$$

in $\rho_D + H_\circ$. Following [3, Theorem 2.2] we have $\rho(F) \in L^\infty(W)$ with $\inf \rho(F) > 0$ and the mapping $\rho(\cdot)$ is $L^2(W) \to H^1(W)$-continuous.

Step 1.2. Given $\rho \in L^\infty(W)$ with $\inf \rho > 0$ it is readily seen that

$$-\nabla \cdot (\rho \nabla F) = 0 \text{ a.e. in } W, \quad F - F_D \in H_\circ$$

has a unique $H^1(W)$-weak solution $F_\circ(\rho)$ — i.e., there is exactly one $F_\circ(\rho) = F \in F_D + H_\circ$ such that (2.5a) holds for all $\varphi \in H_\circ$. Furthermore, due to $0 < \rho < +\infty$ weak minimum/maximum principles allow to deduce $\inf F_D \leq F_\circ(\rho) \leq \sup F_D$.

Step 1.3. We set $T_M(F) = F_\circ(\rho(F))$. Obviously, if $M > \|F_D\|_{L^\infty(W)}$, then T_M will map $\mathsf{C}(M)$ into $\mathsf{C}(M)$. Furthermore, if (F, ρ, V) is a H^1solution of (2.3) with $\mathrm{essinf}_{\mathbf{x} \in D} \rho(\mathbf{x}) > 0$, then there will be an $M > 0$ — e.g. any M with $M > \|F\|_{L^\infty(W)}$ — such that $F \in \mathsf{C}(M)$ and F is a fixed point of T_M.

Step 2. Now we derive an a priori estimate for $V_\circ(\rho(F)^2 - C)$, where here and in the remaining part of Step 2 we keep $F \in L^\infty(W)$ fixed. We recall: $\rho(F)$ is the minimizer of $E(F)$ in $\rho_D + H_\circ$. Since $\rho_D \in \rho_D + H_\circ$ we have

$$E(F)(\rho(F)) \leq E(F)(\rho_D). \tag{A.1}$$

From $\rho_D \in H_b$ we conclude that $E(F)(\rho_D) < +\infty$. Furthermore, for all $\rho \in \rho_D + H_\circ$, we have due to

$$\forall t, \kappa \in [0, +\infty[: \quad t \cdot (\log t - 1 - \kappa) \geq -e^\kappa,$$

$$E(F)(\rho)$$
$$= \varepsilon^2 \int_W |\nabla \rho|^2 \, d\mathbf{x} + \int_W \rho^2 (\log(\rho^2) - 1 + V^* + B - F) \, d\mathbf{x} + \frac{1}{2} \int_W |\nabla V_\circ (\rho^2 - C)|^2 \, d\mathbf{x}$$
$$\geq \varepsilon^2 \int_W |\nabla \rho|^2 \, d\mathbf{x} + \int_W \rho^2 (\log(\rho^2) - 1 - \|V^*\|_{L^\infty(W)} - \|B\|_{L^\infty(W)} - \|F\|_{L^\infty(W)}) \, d\mathbf{x}$$
$$\geq \varepsilon^2 \int_W |\nabla \rho|^2 \, d\mathbf{x} - \text{meas}(W) \exp\Big(\|V^*\|_{L^\infty(W)} + \|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}\Big),$$

where $\text{meas}(W)$ is the Lebesgue measure of W. Utilizing

$$\|\varphi\|_{L^\infty(W)} \leq \|\varphi\|_{H \cap L^\infty(W)} \quad \text{for all } \varphi \in H^1 \cap L^\infty(W)$$

and $\|V_*\|_{L^\infty(W)} \leq \|V_D\|_{L^\infty(W)} \leq \|V_D\|_b$ we obtain

$$E(F)(\rho)$$
$$\geq \varepsilon^2 \int_W |\nabla \rho|^2 \, d\mathbf{x} - \text{meas}(W) \exp\Big(\|V_D\|_b + \|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}\Big)$$
$$= \varepsilon^2 \int_W |\nabla \rho|^2 \, d\mathbf{x} - c_1 \, e^{\|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}},$$

where the constant $c_1 > 0$ depends on $\text{meas}(W)$, $\|V_D\|_{H_b}$, such that via (A.1),

$$\int_W |\nabla \rho(F)|^2 \, d\mathbf{x} \leq \frac{1}{\varepsilon^2} \Big(E(F)(\rho_D) + c_1 \, e^{\|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}}\Big). \qquad \text{(A.2)}$$

In order to obtain an upper estimate for $E(F)(\rho_D)$ we calculate via Remark 2.3-e) and via

$$\forall t \in [0, +\infty[: \quad \log t \leq 1 + t, \quad t \cdot (\log t - 1) \leq t^2,$$

$$E(F)(\rho_D)$$
$$= \varepsilon^2 \int_W |\nabla \rho_D|^2 \, d\mathbf{x} + \int_W \rho_D^2 (\log(\rho_D^2) - 1 + V^* + B - F) \, d\mathbf{x} + \frac{1}{2} \int_W |\nabla V_\circ (\rho_D^2 - C)|^2 \, d\mathbf{x}$$
$$\leq \varepsilon^2 \|\rho_D\|_{H^1(W)}^2 + \int_W \|\rho_D\|_{L^\infty(W)}^4 \, d\mathbf{x}$$
$$\quad + \int_W \|\rho_D\|_{L^\infty(W)}^2 \Big(\|V^*\|_{L^\infty(W)} + \|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}\Big) \, d\mathbf{x}$$
$$\quad + \frac{C_P \text{meas}(W)}{2\lambda^4} \Big(\|\rho_D\|_{L^\infty(W)}^2 + \|C\|_{L^\infty(W)}\Big)^2$$
$$\leq \varepsilon^2 \|\rho_D\|_b^2 + \int_W \|\rho_D\|_b^4 \, d\mathbf{x}$$
$$\quad + \int_W \|\rho_D\|_b^2 \Big(\|V_D\|_b + \|B\|_{L^\infty(W)} + \|F\|_b\Big) \, d\mathbf{x}$$
$$\quad + \frac{C_P \text{meas}(W)}{2\lambda^4} \Big(\|\rho_D\|_b^2 + \|C\|_{L^\infty(W)}\Big)^2,$$

i.e., there is a constant $c_2 > 0$ depending on meas(W), ε, λ, C_P, $\|\rho_D\|_b$, $\|V_D\|_b$, $\|C\|_{L^\infty(W)}$ with

$$E(F)(\rho_D) \leq c_2 \left(1 + \|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}\right)$$
$$\leq c_2 \, e^{\|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}}. \tag{A.3}$$

With the aid of Poincaré's inequality we deduce from (A.2), (A.3),

$$\|\rho(F)\|_{H^1(W)} \leq \|\rho(F) - \rho_D\|_{H^1(W)} + \|\rho_D\|_{H^1(W)}$$
$$\leq \sqrt{1+C_P}\sqrt{\int_W |\nabla(\rho(F)-\rho_D)|^2 \,\mathrm{d}\mathbf{x}} + \|\rho_D\|_b$$
$$\leq \sqrt{1+C_P}\sqrt{\int_W |\nabla\rho(F)|^2 \,\mathrm{d}\mathbf{x} + \int_W |\nabla\rho_D|^2 \,\mathrm{d}\mathbf{x}} + \|\rho_D\|_b$$
$$\leq \sqrt{1+C_P}\left(\sqrt{\int_W |\nabla\rho(F)|^2 \,\mathrm{d}\mathbf{x}} + \sqrt{\int_W |\nabla\rho_D|^2 \,\mathrm{d}\mathbf{x}}\right) + \|\rho_D\|_b$$
$$\leq \sqrt{1+C_P}\sqrt{\int_W |\nabla\rho(F)|^2 \,\mathrm{d}\mathbf{x}} + (1+\sqrt{1+C_P})\|\rho_D\|_b$$
$$\leq \sqrt{1+C_P}\sqrt{\frac{c_2}{\varepsilon^2}e^{\|B\|_{L^\infty(W)}+\|F\|_{L^\infty(W)}} + \frac{c_1}{\varepsilon^2}e^{\|B\|_{L^\infty(W)}+\|F\|_{L^\infty(W)}}}$$
$$+ (1+\sqrt{1+C_P})\|\rho_D\|_b,$$

i.e., there is a constant $c_3 > 0$ depending on meas(W), ε, λ, C_P, $\|\rho_D\|_b$, $\|V_D\|_b$, $\|C\|_{L^\infty(W)}$ such that

$$\|\rho(F)\|_{H^1(W)} \leq c_3 \, e^{\|B\|_{L^\infty(W)}+\|F\|_{L^\infty(W)}}. \tag{A.4}$$

Following [1] there is a constant $c_4 > 0$, just depending on W such that due to $d=1,2$ or $d=3$,

$$\|\rho(F)\|_{L^6(W)} \leq c_4 \|\rho(F)\|_{H^1(W)}, \tag{A.5}$$

and due to [5] there is a constant $c_5 > 0$, just depending on W such that

$$\|V_\circ(\rho(F)^2 - C)\|_{L^\infty(W)} \leq \frac{c_5}{\lambda^2}\|\rho(F)^2 - C\|_{L^3(W)}.$$

We deduce from (A.5) and (A.4),

$$\|V_\circ(\rho(F)^2 - C)\|_{L^\infty(W)} \leq \frac{c_5}{\lambda^2}\left(\|\rho\|_{L^6(W)}^2 + \mathrm{meas}(W)^{1/3}\|C\|_{L^\infty(W)}\right)$$
$$\leq \frac{c_5}{\lambda^2}\left(c_4\|\rho(F)\|_{H^1(W)}^2 + \mathrm{meas}(W)^{1/3}\|C\|_{L^\infty(W)}\right)$$
$$\leq \frac{c_5}{\lambda^2}\left(c_4^2 c_3^2 \, e^{2\|B\|_{L^\infty(W)}+2\|F\|_{L^\infty(W)}} + \mathrm{meas}(W)^{1/3}\|C\|_{L^\infty(W)}\right),$$

i.e., there exists a constant $c_6 \in \mathbb{R}^+$ depending on W, ε, λ, C_P, $\|\rho_D\|_b$, $\|V_D\|_b$, $\|C\|_{L^\infty(W)}$ such that

$$\|V_\circ(\rho(F)^2 - C)\|_{L^\infty(W)} \leq c_6 \, e^{2\|B\|_{L^\infty(W)}+2\|F\|_{L^\infty(W)}}. \tag{A.6}$$

Step 3. Now we derive an a priori estimate on $\|\rho(F)\|_{L^\infty(W)}$, where throughout Step 3 we assume that $F \in L^\infty(W)$ is fixed. Due to Theorem 2.2 in [3] the minimizer $\rho = \rho(F)$ satisfies (2.5b) for all $\varphi \in H_\circ$. A standard monotonicity argument yields the estimates

$$\log\big((\sup\rho(F))^2\big) - \|V\|_{L^\infty(W)} - \|B\|_{L^\infty(W)} - \|F\|_{L^\infty(W)} \leq 0,$$

and

$$\log\big((\inf\rho(F))^2\big) + \|V\|_{L^\infty(W)} + \|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)} \geq 0,$$

such that via $V = V_\circ(\rho(F)^2 - C) + V^*$ and via (A.6),

$$\log\big((\sup\rho(F))^2\big) \leq \|V^*\|_{L^\infty(W)} + c_6\ e^{2\|B\|_{L^\infty(W)} + 2\|F\|_{L^\infty(W)}} + \|B\|_{L^\infty(W)}$$
$$+ \|F\|_{L^\infty(W)},$$
$$\log((\inf\rho(F))^2) \geq -\|V^*\|_{L^\infty(W)} - c_6\ e^{2\|B\|_{L^\infty(W)} + 2\|F\|_{L^\infty(W)}} - \|B\|_{L^\infty(W)}$$
$$- \|F\|_{L^\infty(W)},$$

i.e., there is a constant $c_7 > 0$ depending on W, ε, λ, C_P, $\|\rho_D\|_b$, $\|V_D\|_b$, $\|C\|_{L^\infty(W)}$ such that

$$\exp\big(-c_7 e^{2\|B\|_{L^\infty(W)} + 2\|F\|_{L^\infty(W)}}\big) \leq \rho(F) \leq \exp\big(c_7 e^{2\|B\|_{L^\infty(W)} + 2\|F\|_{L^\infty(W)}}\big). \quad \text{(A.7)}$$

Step 4. We follow the lines of the proofs of Theorems 2.1, 2.2 and Lemma 2.3 in [3] to deduce that $T_M : \mathsf{C}(M) \to H^1(W)$ is $L^2(W) \to L^2(W)$-continuous and T_M maps the convex set $\mathsf{C}(M)$ — which is closed in $L^2(W)$ — into $H^1(W)$ which is precompact in $L^2(W)$. Furthermore, if $M > \|F\|_{L^\infty(W)}$, then - due to the lower estimate on $\rho(F)$ according to (A.7), see Step 1.3 - T_M maps $\mathsf{C}(M)$ into $\mathsf{C}(M)$. By Schauder's Fixed Point Theorem, T_M has in this case a fixed point. Certainly, any fixed point of T_M is a H^1solution of (2.3). Thus, (2.3) has at least one H^1solution.

Step 5. Now let (F, ρ, V) be an arbitrary H^1solution of (2.3). Then there is $M \in \mathbb{R}^+$ with $F \in T_M$ and we have $\rho = \rho(F)$. By (A.7),

$$\rho(F) \leq \exp\big(c_7\ e^{2\|B\|_{L^\infty(W)} + 2\|F\|_{L^\infty(W)}}\big),$$

by (A.4),

$$\|\rho(F)\|_{H^1(W)} \leq c_3\ e^{\|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}}$$

by (A.6),

$$\|V\|_{L^\infty(W)} = \|V_\circ(\rho(F)^2 - C) + V^*\|_{L^\infty(W)}$$
$$\leq c_6\ e^{\|B\|_{L^\infty(W)} + \|F\|_{L^\infty(W)}} + \|V_D\|_{L^\infty(W)},$$

and by easy manipulations of Poisson's equation there is $c_8 > 0$ depending on W, λ, C_P, $\|C\|_{L^\infty(W)}$ such that

$$\|V_\circ(\rho(F)^2 - C)\|_{H^1(W)} \leq c_8\left(1 + \|\rho(F)\|_{L^\infty(W)}^2\right),$$

and due to

$$\|F\|_{L^\infty(W)} \leq \|F_D\|_{L^\infty(W)} \leq \|F_D\|_b,$$

and due to a standard argument we deduce

$$\sqrt{\int_W |\nabla(F - F_D)|^2 \, d\mathbf{x}} \le \frac{\operatorname{esssup} \rho(F)}{\operatorname{essinf} \rho(F)} \sqrt{\int_W |\nabla F_D|^2 \, d\mathbf{x}}.$$

Consequence: there is a constant $c \in \mathbb{R}^+$ depending on W, ε, λ, C_P, $\|\rho_D\|_b$, $\|V_D\|_b$, $\|C\|_{L^\infty(W)}$, $\|F_D\|_b$ such that

$$\|F\|_b + \|\rho\|_b + \|V\|_b \le c \; e^{2e^{\|B\|_{L^\infty(W)}}}.$$

which gives (2.6).

A.2. Proof of Lemma 3.2. We start by computing formally the first and second directional derivative for I at $(\bar{F}, \bar{\rho}) \in H_b \times H_b$ in directions $(F, \rho), (\tilde{F}, \tilde{\rho}) \in H_b \times H_b$ and find

$$\nabla I(\bar{F}, \bar{\rho})(F, \rho) = -\frac{q}{L_1} \int_W \left(2 \bar{\rho} \rho \nabla \bar{F} + \bar{\rho}^2 \nabla F\right) \cdot \vec{e}_1 \, d\mathbf{x} \tag{A.8}$$

and

$$\nabla^2 I(\bar{F}, \bar{\rho})\big((F, \rho), (\tilde{F}, \tilde{\rho})\big) = -\frac{2q}{L_1} \int_W \left(\tilde{\rho} \rho \nabla \bar{F} + \bar{\rho} \rho \nabla \tilde{F} + \bar{\rho} \tilde{\rho} \nabla F\right) \cdot \vec{e}_1 \, d\mathbf{x}. \tag{A.9}$$

To prove that both directional derivatives are Fréchet-derivatives we estimate

$$\left| I(\bar{F} + F, \bar{\rho} + \rho) - I(\bar{F}, \bar{\rho}) - \nabla I(\bar{F}, \bar{\rho})(F, \rho) \right|$$

$$\le \frac{q}{L_1} \int_W \left| \left(\rho^2 \nabla \bar{F} + (2 \bar{\rho} \rho + \rho^2) \nabla F\right) \cdot \vec{e}_1 \right| d\mathbf{x}$$

$$\le c_1 \big(\|\rho\|_{L^4(W)}^2 \|\nabla \bar{F}\|_{L^2(W)} + \|\rho\|_{L^4(W)} \big(1 + 2 \|\bar{\rho}\|_{L^4(W)} \|\rho\|_{L^4(W)}\big) \|\nabla F\|_{L^2(W)} \big),$$

where we have introduced the positive constant $c_1 = q \|\vec{e}_1\|_{L^2(W)} / L_1$. Utilizing Young's inequality and the continuous embedding of $L^\infty(W)$ in $L^4(W)$ there exists a constant $c_2 > 0$ depending on c_1, $\|\nabla \bar{F}\|_{L^2(W)}$, and $\|\bar{\rho}\|_{L^4(W)}$ such that

$$\left| I(\bar{F} + F, \bar{\rho} + \rho) - I(\bar{F}, \bar{\rho}) - \nabla I(\bar{F}, \bar{\rho})(F, \rho) \right| \le c_2 \left(\|\rho\|_{H_b}^2 + \|\rho\|_{H_b}^4 + \|F\|_{H_b}^2 \right).$$

Consequently,

$$\lim_{\|(F, \rho)\|_{H_b \times H_b} \to 0} \frac{|I(\bar{F} + F, \bar{\rho} + \rho) - I(\bar{F}, \bar{\rho}) - \nabla I(\bar{F}, \bar{\rho})(F, \rho)|}{\|(F, \rho)\|_{H_b \times H_b}} = 0.$$

Thus, the first directional derivative of I given by (A.8) is its first Fréchet-derivative. Now we turn to the second derivative. Analogous to the first derivative we estimate

$$\left| \nabla I(\bar{F} + \tilde{F}, \bar{\rho} + \tilde{\rho})(F, \rho) - \nabla I(\bar{F}, \bar{\rho})(F, \rho) - \nabla^2 I(\bar{F}, \bar{\rho})\big((F, \rho), (\tilde{F}, \tilde{\rho})\big) \right|$$

$$\le \frac{q}{L_1} \int_W \left| \left(2 \rho \tilde{\rho} \nabla \tilde{F} + (\tilde{\rho})^2 \nabla F\right) \cdot \vec{e}_1 \right| d\mathbf{x}$$

$$\le \frac{q \|\vec{e}_1\|_{L^2(W)}}{L_1} \left(2 \|\rho\|_{L^4(W)} \|\tilde{\rho}\|_{L^4(W)} \|\nabla \tilde{F}\|_{L^2(W)} + \|\tilde{\rho}\|_{L^4(W)}^2 \|\nabla F\|_{L^2(W)} \right)$$

$$\le \frac{q \|\vec{e}_1\|_{L^2(W)}}{L_1} \left(\|\rho\|_{L^4(W)}^2 \|\tilde{\rho}\|_{L^4(W)}^2 + \|\nabla \tilde{F}\|_{L^2(W)}^2 + \|\tilde{\rho}\|_{L^4(W)}^2 \|\nabla F\|_{L^2(W)} \right),$$

where we have used Young's inequality. Since H_b is continuously (even compactly) embedded in $L^4(W)$, there exists a constant $c_3 > 0$ depending on q, $\|\vec{e}_1\|_{L^2(W)}$, L_1, $\|\rho\|_{L^4(W)}$, and $\|\nabla F\|_{L^2(W)}$ such that

$$\left| \nabla I(\bar{F} + \tilde{F}, \bar{\rho} + \tilde{\rho})(F, \rho) - \nabla I(\bar{F}, \bar{\rho})(F, \rho) - \nabla^2 I(\bar{F}, \bar{\rho})\big((F, \rho), (\tilde{F}, \tilde{\rho})\big) \right|$$
$$\leq c_3 \|(\tilde{F}, \tilde{\rho})\|^2_{H_b \times H_b}.$$

Hence

$$\lim_{\|(\tilde{F}, \tilde{\rho})\|_{H_b \times H_b} \to 0} \frac{\|\nabla I(\bar{F} + \tilde{F}, \bar{\rho} + \tilde{\rho}) - \nabla I(\bar{F}, \bar{\rho}) - \nabla^2 I(\bar{F}, \bar{\rho})(\tilde{F}, \tilde{\rho})\|_{H'_b}}{\|(\tilde{F}, \tilde{\rho})\|_{H_b \times H_b}} = 0.$$

We conclude that the second directional derivative of I is the second Fréchet-derivative.

To prove continuity of the mapping $(\bar{F}, \bar{\rho}) \mapsto \nabla^2 I(\bar{F}, \bar{\rho})$ in the operator norm let us consider $(\bar{F}_1, \bar{\rho}_1), (\bar{F}_2, \bar{\rho}_2) \in H_b \times H_b$. Due to linearity and by similar arguments as used before we obtain for all $(F, \rho), (\tilde{F}, \tilde{\rho}) \in H_b \times H_b$ the estimate

$$|\nabla^2 I(\bar{F}_1, \bar{\rho}_1)\big((F, \rho), (\tilde{F}, \tilde{\rho})\big) - \nabla^2 I(\bar{F}_2, \bar{\rho}_2)\big((F, \rho), (\tilde{F}, \tilde{\rho})\big)|$$
$$\leq \frac{q}{L_1} \|\nabla \bar{F}_1 - \nabla \bar{F}_2\|_{L^2(W)} \|\rho\|_{L^4(W)} \|\tilde{\rho}\|_{L^4(W)}$$
$$+ \frac{q}{L_1} \|\bar{\rho}_1 - \bar{\rho}_2\|_{L^4(W)} \left(\|\rho\|_{L^4(W)} \|\nabla \tilde{F}\|_{L^2(W)} + \|\tilde{\rho}\|_{L^4(W)} \|\nabla F\|_{L^2(W)} \right).$$

We deduce via $\bar{\rho}_1, \bar{\rho}_2 \in L^\infty(W)$ that there is a constant $c_4 > 0$ only depending on W such that

$$\sup\Big\{ \Big| \nabla^2 I(\bar{F}_1, \bar{\rho}_1)\big((F, \rho), (\tilde{F}, \tilde{\rho})\big) - \nabla^2 I(\bar{F}_1, \bar{\rho}_1)\big((F, \rho), (\tilde{F}, \tilde{\rho})\big) \Big| :$$
$$(F, \rho), (\tilde{F}, \tilde{\rho}) \in H_b \times H_b \text{ with } \|(F, \rho)\|_{H_b \times H_b}, \|(\tilde{F}, \tilde{\rho})\|_{H_b \times H_b} \leq 1 \Big\}$$
$$\leq c_4 \left(\|\nabla \bar{F}_1 - \nabla \bar{F}_2\|_{L^2(W)} + \|\bar{\rho}_1 - \bar{\rho}_2\|_{L^\infty(W)} \right) \leq c_4 \|(\bar{F}_1, \bar{\rho}_1) - (\bar{F}_2, \bar{\rho}_2)\|_{H_b \times H_b}.$$

Hence, $\nabla^2 I$ is a (Lipschitz)-continuous function and the claim is proved.

A.3. Proof of Lemma 4.1.   Let $\bar{x} = (\bar{F}, \bar{\rho}, \bar{V}, \bar{u}) \in X$ with $\operatorname{essinf}_W \bar{\rho} > 0$. Since e^4, e^5, e^6 are linear and bounded on X, these operators are Fréchet-differentiable. In fact, for directions $x = (F, \rho, V, u) \in X$ with $\operatorname{essinf}_W(\bar{\rho} + \rho) > 0$ we find

$$\nabla e^4(\bar{x})x = \tau_D(F), \quad \nabla e^5(\bar{x})x = \tau_D(\rho), \quad \nabla e^6(\bar{x})x = \tau_D(V).$$

Moreover, their second derivatives are zero. Let us turn to the operator e^1 whose first directional derivative at $\bar{x}$ in direction x is

$$\langle \nabla e^1(\bar{x})x, \varphi \rangle_{H'_\circ, H_\circ} = \int_W \big(2\bar{\rho}\rho \nabla \bar{F} + \bar{\rho}^2 \nabla F \big) \cdot \nabla \varphi \, \mathrm{d}\mathbf{x} \quad \text{for } \varphi \in H_\circ.$$

Consequently,

$$\|e^1(\bar{x}+x)-e^1(\bar{x})-\nabla e^1(\bar{x})x\|_{H'}$$

$$= \sup_{\|\varphi\|_{H_\circ}=1} \left| \int_W \left(\rho^2(\nabla\bar{F}+\nabla F)+2\bar{\rho}\rho\nabla F\right)\cdot\nabla\varphi\,\mathrm{d}\mathbf{x}\right|$$

$$\leq \sup_{\|\varphi\|_{H_\circ}=1} \|\rho\|^2_{L^\infty(W)}\left(\|\nabla\bar{F}\|_{L^2(W)}+\|\nabla F\|_{L^2(W)}\right)\|\nabla\varphi\|_{L^2(W)}$$

$$+2\sup_{\|\varphi\|_{H_\circ}=1} \|\bar{\rho}\|_{L^\infty(W)}\|\rho\|_{L^\infty(W)}\|\nabla F\|_{L^2(W)}\|\nabla\varphi\|_{L^2(W)}$$

$$\leq \|\rho\|^2_{H_b}\left(\|\nabla\bar{F}\|_{L^2(W)}+\|F\|_{H_b}\right)+2\|\bar{\rho}\|_{L^\infty(W)}\|\rho\|_{H_b}\|F\|_{H_b}$$

$$\leq c_1\left(\|\rho\|^2_{H_b}(1+\|F\|_{H_b})+\|\rho\|_{H_b}\|F\|_{H_b}\right),$$

where the constant $c_1>0$ depends on $\|\nabla\bar{F}\|_{L^2(W)}$ and $\|\bar{\rho}\|_{L^\infty(W)}$. Thus, we have

$$\lim_{\|x\|_X\to0} \frac{\|e^1(\bar{x}+x)-e^1(\bar{x})-\nabla e^1(\bar{x})x\|_{H'}}{\|x\|_X}=0.$$

The directional derivative of $\nabla e^1(\bar{x})x$ at $\bar{x}$ in direction $\tilde{x}=(\tilde{F},\tilde{\rho},\tilde{V},\tilde{u})\in X$, is

$$\langle\nabla^2 e^1(\bar{x})(x,\tilde{x}),\varphi\rangle_{H'_\circ,H_\circ}=2\int_W\left(\tilde{\rho}\rho\nabla\bar{F}+\bar{\rho}\rho\nabla\tilde{F}+\bar{\rho}\tilde{\rho}\nabla F)\right)\cdot\nabla\varphi\,\mathrm{d}\mathbf{x}\quad\text{for }\varphi\in H_\circ.$$

We calculate

$$\|\nabla e^1(\bar{x}+\tilde{x})-\nabla e^1(\bar{x})-\nabla^2 e^1(\bar{x})(\tilde{x},\cdot)\|_{L(X,H')}$$

$$= \sup_{\|x\|_X=1} \|(\nabla e^1(\bar{x}+\tilde{x}))x-\nabla e^1(\bar{x})x-\nabla^2 e^1(\bar{x})(\tilde{x},x)\|_{H'}$$

$$= \sup_{\|x\|_X=1}\sup_{\|\varphi\|_{H_\circ}=1} \left|\langle\nabla e^1(\bar{x}+\tilde{x})x-\nabla e^1(\bar{x})x-\nabla^2 e^1(\bar{x})(x,\tilde{x}),\varphi\rangle_{H'_\circ,H_\circ}\right|$$

$$= \sup_{\|x\|_X=1}\sup_{\|\varphi\|_{H_\circ}=1} \left|\int_W 2\left(\tilde{\rho}\rho\nabla\tilde{F}+\tilde{\rho}^2\nabla F\right)\cdot\nabla\varphi\,\mathrm{d}\mathbf{x}\right|$$

$$\leq 2\sup_{\|x\|_X=1}\left(\|\tilde{\rho}\|_{L^\infty(W)}\|\rho\|_{L^\infty(W)}\|\nabla\tilde{F}\|_{L^2(W;\mathbb{R}^d)}+\|\tilde{\rho}\|^2_{L^\infty(W)}\|\nabla F\|_{L^2(W;\mathbb{R}^d)}\right)$$

$$\leq c_2\|\tilde{x}\|^2_X$$

for a constant $c_2>0$, which depends on embedding constants of $L^\infty(W),L^4(W)$ in H_b. Here, $L(X,H')$ denotes the normed linear space of all bounded linear operators from X to H' supplied with the common norm. Thus,

$$\lim_{\|\tilde{x}\|_X\to0} \frac{\|\nabla e^1(\bar{x}+\tilde{x})-\nabla e^1(\bar{x})-\nabla^2 e^1(\bar{x})(\tilde{x},\cdot)\|_{L(X,H')}}{\|\tilde{x}\|_X}=0.$$

Since the mapping $\bar{x}\mapsto\nabla^2 e^1(\bar{x})$ is linear and bounded, we conclude that $\nabla^2 e^1$ is Lipschitz-continuous.
We proceed by investigating the operator e^2. The first directional derivative has the

form

$$\langle \nabla e^2(\bar{x})x, \varphi \rangle_{H'_\circ, H_\circ} = \int_W \rho(\bar{V} + B(\cdot; \bar{u}) + \log((\bar{\rho})^2) - \bar{F})\varphi \, d\mathbf{x}$$

$$+ \int_W \varepsilon \nabla \rho \cdot \nabla \varphi + (\bar{\rho}(V + \nabla_u B(\cdot; \bar{u})u - F) + 2\rho)\varphi \, d\mathbf{x}$$

for $\varphi \in H_\circ$. We derive

$$\|e^2(\bar{x} + x) - e^2(\bar{x}) - \nabla e^2(\bar{x})x\|_{H'}$$

$$\leq \sup_{\|\varphi\|_{H_\circ}=1} \int_W \Big[\big(\rho V + \rho\big(B(\cdot; \bar{u} + u) - B(\cdot; \bar{u})\big) + 2\rho\big(\log(\bar{\rho} + \rho) - \log(\bar{\rho})\big)\big) \varphi$$

$$+ \big(-\rho F + \bar{\rho}\big(B(\cdot; \bar{u} + u) - B(\cdot; \bar{u}) - \nabla_u B(\cdot; \bar{u})u\big) \varphi$$

$$+ 2\bar{\rho}\Big(\log(\bar{\rho} + \rho) - \log(\bar{\rho}) - \frac{\rho}{\bar{\rho}}\Big)\varphi \Big] d\mathbf{x}$$

$$\leq \|\rho\|_{L^\infty(W)} \Big(\|V\|_{L^2(W)} + \|B(\cdot; \bar{u} + u) - B(\cdot; \bar{u})\|_{L^2(W)} \Big)$$

$$+ \|\rho\|_{L^\infty(W)} \Big(2\|\log(\bar{\rho} + \rho) - \log(\bar{\rho})\|_{L^2(W)} + \|F\|_{L^\infty(W)} \Big)$$

$$+ \|\bar{\rho}\|_{L^\infty(W)} \|B(\cdot; \bar{u} + u) - B(\cdot; \bar{u}) - \nabla_u B(\cdot; \bar{u})u\|_{L^2(W)}$$

$$+ 2\|\bar{\rho}\|_{L^\infty(W)} \Big\|\log(\bar{\rho} + \rho) - \log(\bar{\rho}) - \frac{\rho}{\bar{\rho}}\Big\|_{L^2(W)}.$$

By (**A7**) the mapping B is twice continuously differentiable with respect to the control variable. Thus, there exist constants $c_2, c_3 > 0$ depending on $\bar{u}$ such that

$$\|B(\cdot; \bar{u} + u) - B(\cdot; \bar{u})\|_{L^2(W)} \leq c_2 \|u\|_{\mathbb{R}^\ell}, \qquad (\text{A.10a})$$

$$\big\|B(\cdot; \bar{u} + u) - B(\cdot; \bar{u}) - \nabla_u B(\cdot; \bar{u})u\big\|_{L^2(W)} \leq c_3 \|u\|_{\mathbb{R}^\ell}^2. \qquad (\text{A.10b})$$

Since $\bar{\rho}, \rho \in H_b$ with $\text{essinf}_W \bar{\rho} > 0$ and $\text{essinf}_W(\bar{\rho} + \rho) > 0$ there exist constant $c_3, c_4 > 0$ depending on $\bar{\rho}$ such that

$$\|\log(\bar{\rho} + \rho) - \log(\bar{\rho})\|_{L^2(W)} \leq c_4 \|\rho\|_{H_b}, \qquad (\text{A.10c})$$

$$\Big\|\log(\bar{\rho} + \rho) - \log(\bar{\rho}) - \frac{\rho}{\bar{\rho}}\Big\|_{L^2(W)} \leq c_5 \|\rho\|_{H_b}^2. \qquad (\text{A.10d})$$

From (A.10) and $\|\varphi\|_{L^\infty(W)} \leq \|\varphi\|_{H_b}$ for all $\varphi \in H_b$ it follows that

$$\|e^2(\bar{x} + x) - e^2(\bar{x}) - \nabla e^2(\bar{x})x\|_{H'} \leq c_6 \|\rho\|_{H_b} \big(\|V\|_{H_b} + \|u\|_{\mathbb{R}^\ell} + \|\rho\|_{H_b} + \|F\|_{H_b}\big)$$

$$+ c_6 \|\bar{\rho}\|_{H_b} \Big(\|u\|_{\mathbb{R}^\ell}^2 + \|\bar{\rho}\|_{H_b} \|\rho\|_{H_b}^2\Big),$$

where $c_6 = \max\{1, c_2, c_3 2c_4, 2c_5\} > 0$. Using Young's inequality there is a constant $c_7 > 0$ depending on c_6 and $\bar{\rho}$ satisfying

$$\|e^2(\bar{x} + x) - e^1(\bar{x}) - \nabla e^2(\bar{x})x\|_{H'} \leq c_7 \|x\|_X^2$$

that implies

$$\lim_{\|x\|_X \to 0} \frac{\|e^2(\bar{x} + x) - e^2(\bar{x}) - \nabla e^2(\bar{x})x\|_{H'}}{\|x\|_X} = 0.$$

Hence, the the first directional derivative of e^2 is already the Fréchet-derivative. Next we turn to the second directional derivative of e^2 at $\bar{x}$. In direction $x = (F, \rho, V, u)$, $\tilde{x} = (\tilde{F}, \tilde{\rho}, \tilde{V}, \tilde{u}) \in X$ with $\operatorname{essinf}_W (\bar{\rho} + \tilde{\rho}) > 0$, we find

$$\langle \nabla^2 e^2(\bar{x})(\tilde{x}, x), \varphi \rangle_{H'_\circ, H_\circ} = \int_W \left(\rho \left(\tilde{V} + \nabla_u B(\cdot; \bar{u}) \tilde{u} + \frac{2\tilde{\rho}}{\bar{\rho}} - \tilde{F} \right) + \tilde{\rho} V \right) \varphi \, d\mathbf{x}$$

$$+ \int_W \left(\tilde{\rho}(\nabla_u B(\cdot; \bar{u}) u - F + \tilde{u}^T \nabla_{uu} B(\cdot; \bar{u}) u \bar{\rho}) \right) \varphi \, d\mathbf{x}$$

for $\varphi \in H_\circ$. Then, we obtain

$$\|\nabla e^2(x + \tilde{x}) - \nabla e^2(\bar{x}) - \nabla^2 e^2(\bar{x})(\tilde{x}, \cdot)\|_{L(X, H')}$$

$$= \sup_{\|x\|_X = 1} \sup_{\|\varphi\|_{H_\circ} = 1} \int_W \rho \big(B(\cdot; \bar{u} + \tilde{u}) - B(\cdot; \bar{u}) - \nabla_u B(\cdot; \bar{u}) \tilde{u} \big) \varphi$$

$$+ 2\rho \left(\log(\bar{\rho} + \tilde{\rho}) - \log(\bar{\rho}) - \frac{\tilde{\rho}}{\bar{\rho}} \right) \varphi$$

$$+ \bar{\rho} \big(\nabla_u B(\cdot; \bar{u} + \tilde{u}) u - \nabla_u B(\cdot; \bar{u}) u - \tilde{u}^T \nabla_{uu} B(\cdot; \bar{u}) u \big) \varphi$$

$$+ \tilde{\rho} \big(\nabla_u B(\cdot; \bar{u} + \tilde{u}) u - \nabla_u B(\cdot; \bar{u}) u \big) \varphi \, d\mathbf{x}$$

$$\leq \|B(\cdot; \bar{u} + \tilde{u}) - B(\cdot; \bar{u}) - \nabla_u B(\cdot; \bar{u})\|_{L^2(W; \mathbb{R}^d)} \|\tilde{u}\|_{\mathbb{R}^\ell}$$

$$+ 2 \left\| \log(\bar{\rho} + \tilde{\rho}) - \log(\bar{\rho}) - \frac{\tilde{\rho}}{\bar{\rho}} \right\|_{L^2(W)}$$

$$+ \|\bar{\rho}\|_{L^\infty(W)} \|\nabla_u B(\cdot; \bar{u} + \tilde{u}) - \nabla_u B(\cdot; \bar{u}) - \tilde{u}^T \nabla_{uu} B(\cdot; \bar{u})\|_{L^2(W; \mathbb{R}^d)}$$

$$+ \|\tilde{\rho}\|_{L^\infty(W)} \|\nabla_u B(\cdot; \bar{u} + \tilde{u}) - \nabla_u B(\cdot; \bar{u})\|_{L^2(W; \mathbb{R}^d)}.$$

From (**A7**) we conclude that

$$\|\nabla_u B(\cdot; \bar{u} + \tilde{u}) - \nabla_u B(\cdot; \bar{u}) - \tilde{u}^T \nabla_{uu} B(\cdot; \bar{u})\|_{L^2(W; \mathbb{R}^d)} = o\big(\|\tilde{u}\|_{\mathbb{R}^\ell}\big)$$

so that there is a constant $c_8 > 0$ depending on $\bar{x}$ such that

$$\|\nabla e^2(x + \tilde{x}) - \nabla e^2(\bar{x}) - \nabla^2 e^2(\bar{x})(\tilde{x}, \cdot)\|_{L(X, H')}$$

$$\leq c_8 \left(\|\tilde{u}\|_{\mathbb{R}^\ell}^3 + \|\tilde{\rho}\|_{H_b}^2 + \|\tilde{\rho}\|_{L^\infty(W)} \|\tilde{u}\|_{\mathbb{R}^\ell} \right) + o\big(\|\tilde{u}\|_{\mathbb{R}^\ell}\big) = o\big(\|\tilde{x}\|_X\big).$$

Consequently,

$$\lim_{\|\tilde{x}\|_X \to 0} \frac{\|\nabla e^2(x + \tilde{x}) - \nabla e^2(\bar{x}) - \nabla^2 e^2(\bar{x})(\tilde{x}, \cdot)\|_{L(X, H')}}{\|\tilde{x}\|_X} = 0$$

and the second derivative $\nabla^2 e^2(\bar{x})(\tilde{x}, \cdot)$ is already the second Fréchet-derivative. By (**A7**) the mapping $u \mapsto \nabla_{uu} B(\cdot; u)$ is locally Lipschitz-continuous. Hence, $\nabla^2 e^2(\bar{x})(\tilde{x}, \cdot)$ is locally Lipschitz-continuous as well.

Finally we study the operator e_3. Its directional derivative at the point $\bar{x}$ in any direction $x \in X$ is given by

$$\langle \nabla e^3(\bar{x}) x, \varphi \rangle_{H'_\circ, H_\circ} = \int_W \lambda^2 \nabla V \cdot \nabla \varphi - 2 \bar{\rho} \rho \varphi \, d\mathbf{x} \quad \text{for } \varphi \in H_\circ.$$

Then we estimate

$$\|e^3(\bar{x}+x) - e^3(\bar{x}) - \nabla e^3(\bar{x})x\|_{H'}$$

$$\leq \sup_{\|\varphi\|_{H_\circ}=1} \int_W |\rho^2\varphi|\, d\mathbf{x} \leq \sqrt{\mathrm{meas}(W)}\,\|\rho\|^2_{L^\infty(W)}. \tag{A.11}$$

From (A.11) we directly conclude that ∇e_3 is Fréchet-differentiable and the directional derivative coincides with the first Fréchet-derivative. Setting

$$\langle \nabla^2 e^3(\bar{x})(x,\tilde{x}), \varphi \rangle_{H'_\circ, H_\circ} = -2 \int_W \rho\tilde{\rho}\varphi\, d\mathbf{x}$$

we obtain

$$\|\nabla e^3(\bar{x}+\tilde{x}) - \nabla e^3(\bar{x}) - \nabla^2 e_3(\bar{x})\tilde{x}\|_{L(X,H')} = 0$$

so that e^3 is twice Fréchet-differentiable with second Fréchet-derivative $\nabla^2 e^3$ given above. Since $\nabla^2 e^3(\bar{x})$ does not depend on $\bar{x}$, the second Fréchet-derivative is Lipschitz-continuous on X.

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