



UNIVERSITÀ
DEGLI STUDI
FIRENZE

FLORE

Repository istituzionale dell'Università degli Studi di Firenze

An optimal control problem for the Wigner equation

Questa è la Versione finale referata (Post print/Accepted manuscript) della seguente pubblicazione:

Original Citation:

An optimal control problem for the Wigner equation / Omar Morandi, N.R.. - In: SIAM JOURNAL ON APPLIED MATHEMATICS. - ISSN 1095-712X. - STAMPA. - 84:(2024), pp. 387-411. [10.1137/22M1515033]

Availability:

The webpage <https://hdl.handle.net/2158/1339112> of the repository was last updated on 2024-10-07T07:40:08Z

Published version:

DOI: 10.1137/22M1515033

Terms of use:

Open Access

La pubblicazione è resa disponibile sotto le norme e i termini della licenza di deposito, secondo quanto stabilito dalla Policy per l'accesso aperto dell'Università degli Studi di Firenze (<https://www.sba.unifi.it/upload/policy-oa-2016-1.pdf>)

Publisher copyright claim:

Conformità alle politiche dell'editore / Compliance to publisher's policies

Questa versione della pubblicazione è conforme a quanto richiesto dalle politiche dell'editore in materia di copyright.

This version of the publication conforms to the publisher's copyright policies.

La data sopra indicata si riferisce all'ultimo aggiornamento della scheda del Repository FloRe - The above-mentioned date refers to the last update of the record in the Institutional Repository FloRe

(Article begins on next page)

An optimal control problem for the Wigner equation

Omar Morandi* Nella Rotundo[†] Alfio Borzi[‡] Luigi Barletti[§]

October 27, 2023

Abstract

The Wigner quasi-density function allows a phase-space formulation of statistical quantum mechanics that is of fundamental importance in theoretical investigation and in applications. This work contributes to these tasks with the formulation and analysis of an optimal control problem for the Wigner equation, which describes the time evolution of the quasi-density function.

For this purpose, two possible control mechanisms are considered and, correspondingly, a detailed analysis in weighted Sobolev spaces for the controlled nonhomogeneous Wigner equation is presented. Further theoretical results are reported concerning existence of optimal controls and differentiability of the control-to-state map and of the ensemble cost functional, which allows the derivation of the optimality system that characterizes the optimal controls sought.

Keywords: Wigner equation, Schrödinger equation, Optimal control theory, Ensemble cost functional, Control potentials.

MSC: 35Q93, 49J20, 81Q93

1 Introduction

The works by H. Weyl in [39] and E. Wigner in [40] in the thirties of last century mark the beginning of a continued effort in the development of a statistical formulation of

*O. MORANDI: omar.morandi@unifi.it; Dipartimento di Matematica 'Ulisse Dini', Università di Firenze, Viale Morgagni 67/A, 50134 Firenze, Italy.

[†]N. ROTUNDO: nella.rotundo@unifi.it; Dipartimento di Matematica 'Ulisse Dini', Università di Firenze, Viale Morgagni 67/A, 50134 Firenze, Italy.

[‡]A. BORZI: alfio.borzi@mathematik.uni-wuerzburg.de; Institut für Mathematik, Universität Würzburg, Emil-Fischer-Strasse 30, 97074 Würzburg, Germany.

[§]L. BARLETTI: luigi.barletti@unifi.it; Dipartimento di Matematica 'Ulisse Dini', Università di Firenze, Viale Morgagni 67/A, 50134 Firenze, Italy.

quantum mechanics that is of fundamental importance in the theoretical investigation of quantum mechanical phenomena and related applications.

A distinctive feature of the Weyl-Wigner formulation is the ability to represent a quantum state in phase space, thus allowing to draw a clear connection between quantum and classical mechanics from a statistical perspective. In fact, similar to L.E. Boltzmann's and J.C. Maxwell's statistical approach in classical mechanics, the state of a quantum system is described by a distribution function in phase space that is named Wigner function. However, the Wigner function can assume negative values and for this reason is termed a quasi distribution [12]. On the other hand, we can use the Wigner function in the Weyl-Wigner formulation in the same way of a classical distribution to obtain a complete statistical description of the state of the system in phase space and, in particular, compute expectation values of physical observables [4, 22, 37, 42, 28] .

We recall that in Boltzmann's framework, a time-evolving distribution function provides a statistical description of an ensemble of trajectories. If these classical particles do not interact, then the evolution of the distribution function is governed by the Liouville equation. Specifically, in the case of particles of mass m subject to a potential $U(\mathbf{x})$ and with initial distribution $\rho_0(\mathbf{x}, \mathbf{p})$, the statistical description of the ensemble of the corresponding trajectories is given by the function $\rho(\mathbf{x}, \mathbf{p}, t)$ that solves the following Liouville problem

$$\partial_t \rho + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{x}} \rho - \nabla_{\mathbf{x}} U \cdot \nabla_{\mathbf{p}} \rho = 0, \quad \rho(\mathbf{x}, \mathbf{p}, 0) = \rho_0(\mathbf{x}, \mathbf{p}). \quad (1.1)$$

In quantum mechanics, because of the uncertainty principle, we cannot refer to a phase space trajectory in a classical sense. Nevertheless, the term (quantum) trajectory appears frequently in many different contexts [7, 27, 41] and it acquires its classical meaning in the semiclassical limit. This density distribution is called the Wigner function f , and its evolution is governed by the following Wigner equation (also called the quantum Liouville equation)

$$\partial_t f + \mathbf{p} \cdot \nabla_{\mathbf{x}} f - \Theta_U[f] = 0, \quad (1.2)$$

where, for simplicity, we take the mass $m = 1$.

As in the Liouville problem, a unique $f(\mathbf{x}, \mathbf{p}, t)$ is obtained by specifying an initial distribution $f(\mathbf{x}, \mathbf{p}, 0) = f_0(\mathbf{x}, \mathbf{p})$. In (1.2), the term $\Theta_U[f]$ is a pseudodifferential operator that is specified below (see Eq. (2.3)). However, for quadratic and linear potentials, the Wigner equation reduces to the Liouville equation and, in general, in the semi-classical limit the Liouville equation is recovered regardless of the potential profile.

The ability of the Weyl-Wigner framework to combine concepts that link quantum and classical mechanics from a statistical perspective makes possible to model interaction between quantum and classical systems [13, 43], which is essential in applications. In particular, this framework can also be used to compute quantum corrections to classical results [32, 40, 30, 25] and to investigate open quantum systems and semiconductors; see, e.g., [11, 22, 44]. In applications, the Wigner equation appears in various fields including optics [2, 24], signal processing and pattern recognition [18], quantum transport [21, 36], quantum tunneling phenomena [3, 17, 34, 29, 31], and decoherence [14, 15, 16].

However, while a lot of effort has been put in the analysis and simulation of the Wigner model, much less is known on the formulation and validation of control strategies of the Wigner function that are of fundamental importance in the design of experiments and design of semiconductor devices. For this reason, we would like to contribute to this field of research with the formulation and analysis of optimal control problems governed by the Wigner equation.

In the formulation of control problems for quantum mechanical systems, a control mechanism is implemented in the form of a potential representing, e.g., an electric-magnetic field. A control potential aims at steering the state of a system to perform a desired task. In particular, we can require to reach a given target state and/or optimize the expected value of a given observable. Usually, this action results in a change of energy that necessarily requires a time-dependent potential. Therefore a general setting consists in a total potential $U(\mathbf{x}, t) = U_0(\mathbf{x}) + U_C(\mathbf{x}, t)$, where U_0 represents the (e.g., confining) potential defining the uncontrolled system, and U_C is the control potential. In this framework, the widely considered dipole control mechanism is modelled by the function $\nabla_{\mathbf{x}} U_C(\mathbf{x}, t) = u(t) \mathbf{x}$ where u is a modulating control function; see, e.g., [8] and references therein. Another representative setting is given by a quartic convex potential U_0 and a quadratic concave control potential $U_C(\mathbf{x}, t)$, which allows to split the density for channelling and interference experiments; see, e.g., [20].

In the Weyl-Wigner statistical framework, the purpose of any control mechanism must be formulated in terms of minimizing (or maximizing) expected values of physical observables. In particular, we could require to maximize the expected value of a hermitian operator in phase space A at final time $t = T$ given by

$$\Phi = - \int_{\mathbb{R}^{2n}} A(\mathbf{x}, \mathbf{p}) f(\mathbf{x}, \mathbf{p}, T) \, d\mathbf{x} \, d\mathbf{p} \quad (1.3)$$

(where, with a little abuse of notation, we identify the operator A with its Wigner-Weyl phase-space symbol $A(\mathbf{x}, \mathbf{p})$).

However, in a similar way we can wish to manipulate the distribution function in order to improve the localization of the system at $t = T$ in the neighbourhood of a given point in the phase space denoted with $(\mathbf{x}_T, \mathbf{p}_T)$. For this purpose, we could require to minimize (1.3) with A replaced by V representing a ‘valley’, that is, a function that is locally strictly convex at $(\mathbf{x}_T, \mathbf{p}_T)$ and radially increasing from this point. In particular, we can take

$$V(\mathbf{x}, \mathbf{p}, T) = -C e^{-[(\mathbf{x}-\mathbf{x}_T)^2 + (\mathbf{p}-\mathbf{p}_T)^2]}.$$

Notice that by defining the bottom of a valley in phase space and time as the trajectory $(\mathbf{x}_t, \mathbf{p}_t)$, $t \geq 0$, we can also aim at steering the quantum system such that the distribution function $f(\mathbf{x}, \mathbf{p}, t)$ concentrates on this trajectory along the time evolution. Thus, we would consider the minimisation of the following objective

$$\Psi = \int_0^T \int_{\mathbb{R}^{2n}} V(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{p}, t) \, d\mathbf{x} \, d\mathbf{p} \, dt.$$

This modelling strategy has been introduced only recently in [10], and further developed and analyzed in, e.g., [1, 5, 6, 35] for the optimal control of a Liouville equation,

a linear Boltzmann equation, and a Fokker-Planck equation. As proposed in [10], optimal control problems governed by continuity equations and involving expected value functionals are called ensemble optimal control problems.

We remark that, in addition to defining the purpose of the control, we need to measure the cost of its action that should be kept as small as possible. For this purpose, an appropriate norm of the control function U_C is added to the functional above, thus defining a cost functional to be minimized with the additive structure $J = \Phi + \Psi + \|U_C\|^2$.

Our purpose is to formulate and analyze a class of ensemble optimal control problems governed by the Wigner equation in phase space. In this way, we extend previous results [1] for similar problems governed by a generic Liouville equation in the $\mathbf{x}$ space. However, this extension results challenging because of the presence of the pseudodifferential operator Θ_U , and requires to considerably improve upon known results to allow a complete characterization of solutions to our optimal control problems.

For this reason, we present a novel detailed analysis of the Wigner equation with a time-varying control potential in a functional setting where the initial condition and the solution are defined in weighted Sobolev spaces. In this way, we provide the appropriate functional framework for proving existence of optimal controls and for characterizing these controls by first-order optimality conditions. Therefore we present a complete analysis of Fréchet differentiability of the Wigner equation and of the cost functional, and derive the optimality system that is required for developing optimization procedures for solving optimal control problems [9].

In the next section, we introduce the Wigner density function and the equation that governs its time evolution. In this model, we identify two possible control mechanisms. In Section 3, we present novel theoretical results in weighted Sobolev spaces for a controlled nonhomogeneous Wigner model. In particular, we discuss existence and regularity of solutions for different initial conditions. These results are essential for the analysis presented in Section 4 concerning continuity and differentiability of the control-to-state map. Section 5 is devoted to the formulation of ensemble optimal control problems governed by the Wigner equation. In this section, we prove existence of optimal controls. In Section 6, we discuss Fréchet differentiability of the optimal control problem, and derive the optimality system that characterizes the optimal controls sought. A section of conclusion follows and a final Appendix contains a postponed proof.

2 The Wigner equation

The Wigner equation governs the evolution of the Wigner function of a quantum mechanical system in the phase space coordinates $(\mathbf{x}, \mathbf{p})$. The starting point for the construction this function is the quantum density matrix [19, 37]. The hermitian density matrix $\rho(\mathbf{x}, \mathbf{y}, t)$ can be considered as a generalization of Schrödinger's wavefunctions, since it accommodates both pure and mixed quantum states. The Wigner function

represents the inverse Weyl-Wigner transform of the density ρ as follows

$$f(\mathbf{x}, \mathbf{p}, t) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \rho\left(\mathbf{x} + \frac{\hbar\boldsymbol{\eta}}{2}, \mathbf{x} - \frac{\hbar\boldsymbol{\eta}}{2}, t\right) e^{-i\mathbf{p}\cdot\boldsymbol{\eta}} d\boldsymbol{\eta}. \quad (2.1)$$

A direct consequence of this definition is that f is real valued.

Based on this construction, the Wigner equation is obtained starting from the Schrödinger equation [37]. We have

$$\partial_t f(\mathbf{x}, \mathbf{p}, t) + \mathbf{p} \cdot \nabla_{\mathbf{x}} f - \Theta_U[f] = 0, \quad (2.2)$$

where the skew-symmetric pseudodifferential operator is defined by

$$\begin{aligned} \Theta_U[f](\mathbf{x}, \mathbf{p}, t) &\doteq \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \delta U(\mathbf{x}, \boldsymbol{\eta}, t) f(\mathbf{x}, \mathbf{p}', t) e^{-i(\mathbf{p}-\mathbf{p}')\cdot\boldsymbol{\eta}} d\mathbf{p}' d\boldsymbol{\eta} \\ &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \delta U(\mathbf{x}, \boldsymbol{\eta}, t) \widehat{f}(\mathbf{x}, \boldsymbol{\eta}, t) e^{-i\mathbf{p}\cdot\boldsymbol{\eta}} d\boldsymbol{\eta} \\ &= \mathcal{F}_{\boldsymbol{\eta}} \left(\delta U \widehat{f} \right) (\mathbf{x}, \mathbf{p}, t), \end{aligned} \quad (2.3)$$

$\mathcal{F}_{\boldsymbol{\eta}}$ denotes Fourier transform, and

$$\delta U(\mathbf{x}, \boldsymbol{\eta}, t) \doteq \frac{1}{i\hbar} \left[U\left(\mathbf{x} + \frac{\hbar\boldsymbol{\eta}}{2}\right) - U\left(\mathbf{x} - \frac{\hbar\boldsymbol{\eta}}{2}\right) \right]. \quad (2.4)$$

Notice that (2.2) conserves the quasiprobability in the sense that if the initial density f_0 of the system is normalized to one, then the following holds

$$\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} d\mathbf{x} = 1, \quad t \geq 0.$$

However, although we could choose an initial configuration such that $f_0(\mathbf{x}, \mathbf{p}) \geq 0$, during its evolution the Wigner function can locally take negative values. On the other hand, it cannot take on arbitrary large values since it holds $|f(\mathbf{x}, \mathbf{p}, t)| \leq 2/\hbar$.

In quantum mechanics, a control mechanism is usually implemented by a control potential U_C that is added to the potential of the uncontrolled system U_0 ; see, e.g., [8]. The uncontrolled potential U_0 is typically a confinement potential. Our analysis focuses on a class of bounded U_0 , for example a (smooth) potential well. From the mathematical point of view, the confining character of U_0 is not important; from the physical point of view the confinement is obtained by creating a deep enough well (e.g. by means of suitable electrostatic fields).

Further, we choose a class of control potentials that includes a transport potential such that $\nabla_{\mathbf{x}} U_C(\mathbf{x}, t) = \mathbf{u}(t)$, and a dipole control given by $\nabla_{\mathbf{x}} U_C(\mathbf{x}, t) = \mathbf{x} \circ \mathbf{v}(t)$, where the symbol $\circ$ denotes the Hadamard product in multidimensions. We remark that the latter is omnipresent in quantum optimal control in the Schrödinger framework, whereas the former is typical in open-loop control problems governed by dynamical systems. Due to the relatively easy implementation, dipole fields are employed in many experiments

in which particles are confined at the atomic scale. The experimental feasibility of the control mechanism is at the basis of our choice of considering external dipole field as control mechanisms to quantum dynamics. The control strategy can be easily understood by simple consideration on the statistical mechanics of the particle ensemble. Assuming the initial f_0 to be a Gaussian and $U_0 = 0$, one can verify that the transport potential acts on the mean of the position of an ensemble, whereas the dipole control allows to manipulate the variance; see, e.g., [10] in the case of the classical Liouville equation. For our analysis, we make the following assumptions:

(A.1) **Assumption on the confinement potential:** U_0 is bounded and fixed

$$U_0(\mathbf{x}) \in C_b^{2k}(\mathbb{R}_x^n), \quad (2.5)$$

where $k \in \mathbb{N}$, and $C_b^{2k}(\mathbb{R}_x^n)$ denotes the subspace of the space $C^{2k}(\mathbb{R}_x^n)$ of all $2k$ -times continuously differentiable functions, formed by functions which are uniformly bounded together with all their derivatives up to the order $2k$.

(A.2) **Assumption on the control potential:** U_C is a dipole-type control

$$U_C(\mathbf{x}, t) \doteq \sum_{i=1}^n x_i u_i(t) + \sum_{i=1}^n \frac{x_i^2}{2} v_i(t). \quad (2.6)$$

with $k \geq 0$, $\mathbf{u} = (u_1, \dots, u_n)$ and $\mathbf{v} = (v_1, \dots, v_n)$ are the control functions. We also define the control pair $\mathbf{w} = (\mathbf{u}, \mathbf{v})$, and assume that it belongs to the following space of admissible controls:

$$\mathcal{U} \doteq \left\{ \mathbf{w} := (\mathbf{u}, \mathbf{v}) \in H^1([0, T]; \mathbb{R}^n) \times H^1([0, T]; \mathbb{R}^n) \right\}. \quad (2.7)$$

We remark that Θ_U is linear in U , and, since U_C is quadratic, the contribution of the control potential to the Wigner equation results in the classical expression

$$\Theta_{U_C}[f] = [\mathbf{u}(t) + (\mathbf{x} \circ \mathbf{v}(t))] \cdot \nabla_{\mathbf{p}} f. \quad (2.8)$$

In order to express the dependence of the control potential on the control functions we refer to the control potential as $U_C(\mathbf{w})$ which coincides with $U_C(\mathbf{x}, t)$, with a little abuse of notation.

3 Analysis of the Wigner function in a weighted space

One of our contribution to the formulation of optimal control problems with the Wigner model is the analysis of this model with the given time-dependent unbounded control potentials. For this reason, we have to extend to the non-autonomous case, the results of existence and regularity for the Wigner equation with time-independent potential U (see, e.g., [33, 26]). On the other hand, the presence of the confining potential requires to further develop the theory in [6] on the optimal control of the classical Liouville

equation in the space of coordinates. Moreover, as illustrated below, the characterization of optimal controls leads to the formulation of an optimality system that involves the optimization adjoint of the Wigner equation, which has the same structure of the Wigner equation but includes a source term. Therefore we study the following nonhomogeneous Cauchy problem for the Wigner function

$$\begin{cases} \partial_t f + \mathbf{p} \cdot \nabla_{\mathbf{x}} f - \Theta_U[f] = g, & \text{in } \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n \times [0, T] \\ f|_{t=0} = f_0, & \text{on } \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n. \end{cases} \quad (3.1)$$

In order to accommodate the use of unbounded controls and allow the analysis of (3.1) and of the resulting optimality system, we choose, as in [6], weighted Sobolev spaces that provide the appropriate functional setting.

Notation and definitions

Throughout the paper, we use the notation $\mathbb{R}^{2n} := \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n$ and, when it is clear from the context, we omit to write this space. For example, if $W(\mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n)$ is a generic Sobolev space on $\mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n$, we may denote it only with W .

Definition 3.1. *Let $(m, k) \in \mathbb{N}^2$. We define the space $H_k^m(\mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n)$ in the following way:*

$$H_k^0 \doteq L_k^2 \doteq \left\{ f \in L^2 \mid (|\mathbf{x}| + |\mathbf{p}|)^k f \in L^2 \right\},$$

The space L_k^2 is endowed with the following norm:

$$\|f\|_{L_k^2} \doteq \left(\int_{\mathbb{R}^{2n}} (1 + |\mathbf{x}|^k + |\mathbf{p}|^k)^2 f^2 \, d\mathbf{x} \, d\mathbf{p} \right)^{\frac{1}{2}}.$$

The space H_k^1 is endowed with the following norm:

$$\|f\|_{H_k^1} \doteq \left(\int_{\mathbb{R}^{2n}} (1 + |\mathbf{x}|^k + |\mathbf{p}|^k)^2 (f^2 + (\nabla_{\mathbf{x}} f)^2 + (\nabla_{\mathbf{p}} f)^2) \, d\mathbf{x} \, d\mathbf{p} \right)^{\frac{1}{2}}.$$

Finally, for $m \geq 1$, we set

$$H_k^m \doteq \left\{ f \in H^m \cap H_k^{m-1} \mid (|\mathbf{x}|^k + |\mathbf{p}|^k) D^\alpha f \in L^2(\mathbb{R}^n) \quad \forall |\alpha| = m \right\}.$$

and

$$\|f\|_{H_k^m}^2 \doteq \sum_{|\alpha| \leq m} \left\| (1 + |\mathbf{x}|^k + |\mathbf{p}|^k) D^\alpha f \right\|_{L^2}^2.$$

Notice that, $H_k^m \subset H^m$ for all m and k in $\mathbb{N}$.

In the main part of this section, we present a detailed analysis of the solution to (3.1) in H_k^m spaces assuming $f_0 \in H_k^m$, $m = 0, 1, 2$, $k \in \mathbb{N}$, and a generic source term that satisfies the following:

(A.3) **Assumption on the nonhomogeneous term**

$$g \in L^1 \left([0, T]; H_k^2 \left(\mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n \right) \right). \quad (3.2)$$

(A.4) **Assumption on the initial density:** $f_0 \in H_k^m$, for $m \in \{0, 1, 2\}$, $k \in \mathbb{N}$ fixed, is nonnegative, bounded in the sense $|f_0(\mathbf{x}, \mathbf{p})| \leq 2/h$, and normalized:

$$\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f_0(\mathbf{x}, \mathbf{p}) \, d\mathbf{p} \, d\mathbf{x} = 1. \quad (3.3)$$

In particular, we remark that the bound $|f(\mathbf{x}, \mathbf{p}, t)| \leq 2/h$ follows from (2.1). In fact, every mixed-state density matrix $\rho(x, y, t)$ can be decomposed into a convex combination of pure-state density matrices $\psi(x, t)\bar{\psi}(y, t)$, for which the bound follows directly from the Schwartz inequality (see [12]).

Next, we discuss our problem in the L_k^2 space. Later, we use this result to prove similar estimates in the H_k^1 norm. Finally, we present our results in the H_k^2 space, which will be used in the next sections.

Lemma 3.1 (L_k^2 estimate). *Let $k \in \mathbb{N}$, $T > 0$, and the assumption (A.1)-(A.4) be satisfied with $f_0 \in L_k^2$. Then there exists a unique solution $f \in C([0, T]; L_k^2)$ to the problem (3.1) and the following estimate holds true for any $t \in [0, T]$*

$$\begin{aligned} \|f(\cdot, \cdot, t)\|_{L_k^2} &\leq \left(\|f_0\|_{L_k^2} + 3 \int_0^t \|g(\cdot, \cdot, \tau)\|_{L_k^2} \, d\tau \right) \\ &\times \exp \left(\frac{3k}{2} \int_0^t \left(1 + \sum_i^n (|u_i| + |v_i|) \right) \, d\tau + K_0 t \right). \end{aligned} \quad (3.4)$$

where we have defined

$$K_0 \doteq \frac{6}{\hbar} \left(1 + \left(\frac{\hbar^2}{2} \right)^k \right) \|U_0\|_{C_b^{2k}}. \quad (3.5)$$

The proof of Lemma 3.1 is postponed to Appendix A. This result is now used to prove the main theorems about the Cauchy problem (3.1).

Theorem 3.1 (H_k^1 estimate). *Let $k \in \mathbb{N}$, $T > 0$, and the assumption (A.1)-(A.4) be satisfied with $f_0 \in H_k^1$. Then there exists a unique solution $f \in C([0, T]; H_k^1)$ to problem (3.1), and the following estimate holds true for any $t \in [0, T]$*

$$\begin{aligned} \|f(\cdot, \cdot, t)\|_{H_k^1} &\leq \left(\|f_0\|_{H_k^1} + \alpha \int_0^t \|g(\cdot, \cdot, \tau)\|_{H_k^1} \, d\tau \right) \\ &\times \exp \left(C \int_0^t \left(|\mathbf{u}(\tau)| + |\mathbf{v}(\tau)| + \|U_0(\tau)\|_{C_b^{2k+1}} \right) \, d\tau + C \frac{t}{2} \right), \end{aligned} \quad (3.6)$$

where $\alpha = 9\sqrt{2n+1}$.

Proof: We proceed as in the proof of Lemma 3.1. We take the derivative of the nonhomogeneous Wigner equation (3.1) with respect to space, we multiply by $(1 + |\mathbf{p}|^{2k} + |\mathbf{x}|^{2k}) \frac{\partial f}{\partial x_i}$ and we integrate. This yields

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^{2n}} (1 + r^{2k}) \left(\frac{\partial f}{\partial x_i} \right)^2 d\mathbf{x} d\mathbf{p} \leq \\ & \frac{k}{2} \left(1 + \sum_{j=1}^n (|u_j| + |v_j|) \right) \int_{\mathbb{R}^{2n}} (1 + r^{2k}) \left(\frac{\partial f}{\partial x_i} \right)^2 d\mathbf{x} d\mathbf{p} \\ & + \frac{k}{2} |v_i| \int_{\mathbb{R}^{2n}} (1 + r^{2k}) f^2 d\mathbf{x} d\mathbf{p} \\ & + \|U_0\|_{C_b^{2k+1}} \frac{2}{\hbar} \left(1 + \left(\frac{\hbar^2}{2} \right)^k \right) \int_{\mathbb{R}^{2n}} (1 + r^{2k}) \left[\left(\frac{\partial f}{\partial x_i} \right)^2 + f^2 \right] d\mathbf{x} d\mathbf{p} \\ & + \int_{\mathbb{R}^{2n}} (1 + r^{2k}) \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial x_i} d\mathbf{x} d\mathbf{p} , \end{aligned}$$

where $r^k = |\mathbf{p}|^k + |\mathbf{x}|^k$. After straightforward calculations we obtain

$$\frac{1}{6} \frac{d}{dt} \|\nabla_{\mathbf{x}} f\|_{L_k^2}^2 \leq K_1 \left(\|\nabla_{\mathbf{x}} f\|_{L_k^2}^2 + \|f\|_{L_k^2}^2 \right) + \sqrt{2n+1} \|\nabla_{\mathbf{x}} f\|_{L_k^2} \|\nabla_{\mathbf{x}} g\|_{L_k^2} , \quad (3.7)$$

where

$$K_1 = k \left(1 + \sum_j^n (|u_j| + |v_j|) \right) + \|U_0\|_{C_b^{2k+1}} \frac{2}{\hbar} \left(1 + \left(\frac{\hbar^2}{2} \right)^k \right) ,$$

and we have used $\sum_i \sqrt{a_i} \leq \sqrt{2n+1} \sqrt{\sum_i a_i}$. We apply a similar procedure to the derivative with respect to the momentum of the Wigner function: proceeding as above but with the p_j -derivative, we get

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^{2n}} (1 + r^{2k}) \left(\frac{\partial f}{\partial p_i} \right)^2 d\mathbf{x} d\mathbf{p} \\ & \leq \int_{\mathbb{R}^{2n}} (1 + r^{2k}) \left(\frac{k}{2} \left(\frac{\partial f}{\partial p_i} \right)^2 + \left| \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial p_i} \right| + \left| \frac{\partial f}{\partial p_i} \frac{\partial f}{\partial x_i} \right| \right) d\mathbf{x} d\mathbf{p} \\ & + \left| \int_{\mathbb{R}^{2n}} (1 + r^{2k}) \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_0+U_C}[f] d\mathbf{x} d\mathbf{p} \right| . \end{aligned}$$

We study the term $A_C^i \doteq \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^{2k} + |\mathbf{x}|^{2k}) \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_C}[f] d\mathbf{x} d\mathbf{p}$. We use (2.8) and note that

$$\int_{\mathbb{R}^{2n}} \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_C}[f] d\mathbf{p} = \int_{\mathbb{R}^{2n}} \frac{1}{2} \frac{\partial}{\partial p_i} \left(\mathbf{u} \cdot \nabla_{\mathbf{p}} f^2 + \sum_j x_j v_j \frac{\partial f^2}{\partial p_j} \right) d\mathbf{p} = 0 .$$

We have

$$\sum_i |A_C^i| \leq C \frac{n^2}{2} k \left(|\mathbf{u}| + \max_j |v_j| \right) \left(\|\nabla_{\mathbf{p}} f\|_{L_k^2}^2 + \|f\|_{L_k^2}^2 \right).$$

where we have used

$$\begin{aligned} & \sum_i \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_C}[f] \, d\mathbf{p} \\ &= - \sum_i k \int_{\mathbb{R}^{2n}} p_i |\mathbf{p}|^{2(k-1)} \left(\mathbf{u} \cdot \nabla_{\mathbf{p}} f^2 + \sum_j x_j v_j \frac{\partial f^2}{\partial p_j} \right) d\mathbf{p}. \end{aligned}$$

Next, we consider the term containing the confining potential:

$$\int_{\mathbb{R}^{2n}} \left(1 + |\mathbf{p}|^{2k} + |\mathbf{x}|^{2k} \right) \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_0}[f] \, d\mathbf{x} \, d\mathbf{p}.$$

We write

$$\int_{\mathbb{R}^n} \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_0}[f] \, d\mathbf{p} = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \left| \widehat{f}(\mathbf{x}, \boldsymbol{\eta}) \right|^2 (-\eta_i^2) \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \, d\boldsymbol{\eta},$$

so that we have

$$\begin{aligned} & \sum_i \left| \int_{\mathbb{R}^{2n}} \left(1 + |\mathbf{x}|^{2k} \right) \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_0}[f] \, d\mathbf{p} \, d\mathbf{x} \right| \\ & \leq 2 \|U_0\|_{L^\infty(\mathbb{R}_{\mathbf{x}}^n)} \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \left(1 + |\mathbf{x}|^{2k} \right) \left| \widehat{f}(\mathbf{x}, \boldsymbol{\eta}) \right|^2 |\boldsymbol{\eta}|^2 \, d\boldsymbol{\eta} \, d\mathbf{x} \\ & = 2 \|U_0\|_{L^\infty(\mathbb{R}_{\mathbf{x}}^n)} \int_{\mathbb{R}^{2n}} \left(1 + |\mathbf{x}|^{2k} \right) |\nabla_{\mathbf{p}} f|^2 \, d\mathbf{p} \, d\mathbf{x}. \end{aligned}$$

Finally, let us consider the term containing the momentum

$$\begin{aligned} & \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_0}[f] \, d\mathbf{x} \, d\mathbf{p} \\ &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{3n}} \frac{\partial f(\mathbf{x}, \mathbf{p})}{\partial p_i} (-i\eta_i) \overline{\widehat{f}(\mathbf{x}, \boldsymbol{\eta})} \delta U_0(\mathbf{x}, \boldsymbol{\eta}) |\mathbf{p}|^{2k} e^{-i\mathbf{p} \cdot \boldsymbol{\eta}} \, d\boldsymbol{\eta} \, d\mathbf{x} \, d\mathbf{p} \\ &= \int_{\mathbb{R}^{2n}} \left| \widehat{f}(\mathbf{x}, \boldsymbol{\eta}) \right|^2 (i\eta_i) \left(\sum_j^n -\frac{\partial^2}{\partial \eta_j^2} \right)^k (-i\eta_i) \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \, d\boldsymbol{\eta} \, d\mathbf{x}. \end{aligned}$$

Note that

$$\begin{aligned} & \left(\sum_j^n -\frac{\partial^2}{\partial \eta_j^2} \right)^k (-i\eta_i) \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \\ &= (-i\eta_i) \left(\sum_j^n -\frac{\partial^2}{\partial \eta_j^2} \right)^k \delta U_0(\mathbf{x}, \boldsymbol{\eta}) + \sum C \partial_{\eta}^{2k-1} \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \\ &= (-i\eta_i) \left(\frac{\hbar}{2} \right)^k \left(\sum_j^n -\frac{\partial^2}{\partial x_j^2} \right)^k \delta^+ U_0(\mathbf{x}, \boldsymbol{\eta}) + \sum C' \partial_x^{2k-1} \delta^+ U_0(\mathbf{x}, \boldsymbol{\eta}), \end{aligned}$$

where we have defined $\delta^+ U_0 \doteq \frac{1}{i\hbar} \left[U \left(\mathbf{x} + \frac{\hbar \boldsymbol{\eta}}{2} \right) + U \left(\mathbf{x} - \frac{\hbar \boldsymbol{\eta}}{2} \right) \right]$. Now, we can estimate

$$\begin{aligned} & \left| \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_0}[f] \, d\mathbf{x} \, d\mathbf{p} \right| \leq \\ & \left(\frac{\hbar}{2} \right)^{k-1} \|U_0\|_{C_b^{2k}(\mathbb{R}_{\mathbf{x}}^n)} \int_{\mathbb{R}^{2n}} \left| \widehat{f}(\mathbf{x}, \boldsymbol{\eta}) \right|^2 (\eta_i^2) \, d\boldsymbol{\eta} \, d\mathbf{x} \\ & + C \|U_0\|_{C_b^{2k-1}(\mathbb{R}_{\mathbf{x}}^n)} \int_{\mathbb{R}^{2n}} \left| \widehat{f}(\mathbf{x}, \boldsymbol{\eta}) \right|^2 (-i\eta_i) \, d\boldsymbol{\eta} \, d\mathbf{x} . \end{aligned}$$

Putting together the estimation for U_0 and U_C , we have

$$\begin{aligned} \left| \int_{\mathbb{R}^{2n}} \left(1 + r^{2k} \right) \frac{\partial f}{\partial p_i} \frac{\partial}{\partial p_i} \Theta_{U_0+U_C}[f] \, d\mathbf{x} \, d\mathbf{p} \right| & \leq C \left(|\mathbf{u}| + |\mathbf{v}| + \|U_0\|_{C_b^{2k}(\mathbb{R}_{\mathbf{x}}^n)} \right) \\ & \times \left(\|\nabla_{\mathbf{p}} f\|_{L_k^2}^2 + \|f\|_{L_k^2}^2 \right) . \end{aligned}$$

Using the previous estimates we obtain

$$\begin{aligned} \frac{1}{6} \frac{d}{dt} \|\nabla_{\mathbf{p}} f\|_{L_k^2}^2 & \leq \frac{1}{2} \|\nabla_{\mathbf{x}} f\|_{L_k^2}^2 \\ & + C \left(1 + |\mathbf{u}| + |\mathbf{v}| + \|U_0\|_{C_b^{2k}(\mathbb{R}_{\mathbf{x}}^n)} \right) \left(\|\nabla_{\mathbf{p}} f\|_{L_k^2}^2 + \|f\|_{L_k^2}^2 \right) \\ & + \sqrt{2n+1} \|\nabla_{\mathbf{p}} f\|_{L_k^2} \|\nabla_{\mathbf{p}} g\|_{L_k^2} . \end{aligned} \tag{3.8}$$

Summing up (3.8), (3.7) and (A.7), we get

$$\frac{1}{6} \frac{d}{dt} \|f\|_{H_k^1}^2 \leq K_2 \|f\|_{H_k^1}^2 + 3\sqrt{2n+1} \|f\|_{H_k^1} \|g\|_{H_k^1} ,$$

where

$$K_2 \doteq \frac{1}{3} K + K_1 + \frac{1}{2} + C \left(1 + |\mathbf{u}| + |\mathbf{v}| + \|U_0\|_{C_b^{2k}(\mathbb{R}_{\mathbf{x}}^n)} \right) .$$

For the sake of compactness, we write $K_2 \doteq C + C(|\mathbf{u}| + |\mathbf{v}| + \|U_0\|_{C_b^{2k+1}})$, which yields

$$\frac{d}{dt} \|f\|_{H_k^1} \leq 3K_2 \|f\|_{H_k^1} + 9\sqrt{2n+1} \|g\|_{H_k^1} .$$

□

Theorem 3.2 (H_k^2 norm). *Let $k \in \mathbb{N}$, $T > 0$, and the assumption (A.1)-(A.4) be satisfied with $f_0 \in H_k^2$. Then there exists a unique solution $f \in C([0, T]; H_k^2)$ to the problem (3.1) and the following estimate holds true for any $t \in [0, T]$*

$$\begin{aligned} \|f(\cdot, \cdot, t)\|_{H_k^2} & \leq \left(\|f_0\|_{H_k^2} + C \int_0^t \|g(\cdot, \cdot, \tau)\|_{H_k^2} \, d\tau \right) \times \\ & \exp \left(C \int_0^t \left(|\mathbf{u}(\tau)| + |\mathbf{v}(\tau)| + \|U_0(\tau)\|_{C_b^{2k+2}} \right) \, d\tau + C \frac{t}{2} \right) , \end{aligned}$$

or, in a more compact form,

$$\|f(\cdot, \cdot, T)\|_{H_k^2} \leq \left(\|f_0\|_{H_k^2} + C \|g\|_{L^1([0, T]; H_k^2)} \right) \times \exp \left(C \left(\|\mathbf{u} + \mathbf{v}\|_{L^1([0, T]; \ell_1^n)} + \|U_0\|_{L^1([0, T]; C_b^{2k+2})} + T \right) \right), \quad (3.9)$$

where ℓ_1^n indicates the L^1 norm in $\mathbb{R}^n$.

The proof of Theorem 3.2 follows similar steps to that of Theorem 3.1, so we defer it to Appendix A.

4 Analysis of the control-to-state map

Our analysis has shown that, for a fixed initial condition and given control functions, a unique state of the quantum system, represented by its Wigner function, is obtained. This correspondence defines a control-to-state map. In this section, we prove that this map is continuous and differentiable.

We assume a fixed initial condition $f_0 \in H_k^m$, $m = 0, 1, 2$, and introduce the control-to-state map G , defined by

$$G : \mathcal{U} \longrightarrow L^\infty([0, T]; H_k^m), \quad \mathbf{w} \mapsto f := G(\mathbf{w}),$$

where f is the unique solution to the Cauchy problem (3.1), for the given pair of admissible control functions $\mathbf{w} = (\mathbf{u}, \mathbf{v})$. We have

Lemma 4.1. *Let $k \in \mathbb{N}$ and $T > 0$ fixed. Let $\mathbf{w} \doteq (\mathbf{u}, \mathbf{v})$ and $\tilde{\mathbf{w}} \doteq (\tilde{\mathbf{u}}, \tilde{\mathbf{v}})$ be two admissible pairs of essentially bounded control functions; let U_C and $\tilde{U}_C$ be the corresponding control potentials. Denote with $\delta G \doteq G(\mathbf{w}) - G(\tilde{\mathbf{w}})$ the difference of the states resulting with $\mathbf{w}$ and $\tilde{\mathbf{w}}$, respectively. We assume that (A.1), (A.3) are satisfied and $f_0 \in H_k^2$, and we define*

$$K = K(\mathbf{u} + \mathbf{v}; f_0, g, U_0) \doteq C \left(\|f_0\|_{H_k^2} + C \|g\|_{L^1([0, T]; H_k^2)} \right) \times \exp \left(C \left(\|\mathbf{u} + \mathbf{v}\|_{L^1([0, T]; \ell_1^n)} + \|U_0\|_{L^1([0, T]; C_b^{2k+2})} + T \right) \right). \quad (4.1)$$

Then the following estimate holds true for any $t \in [0, T]$

$$\|\delta G(\cdot, \cdot, t)\|_{H_{k-1}^1} \leq K \int_0^t \left(|\mathbf{u} - \tilde{\mathbf{u}}|^2 + |\mathbf{v} - \tilde{\mathbf{v}}|^2 \right)^{\frac{1}{2}} dt, \quad (4.2)$$

Proof: From the linearity of the Wigner equation, we find that δG satisfies

$$\begin{cases} \partial_t \delta G + \mathbf{p} \cdot \nabla_{\mathbf{x}} \delta G - \Theta_{U_0 + U_C}[\delta G] = \Theta_{U_C - \tilde{U}_C}[G(\tilde{\mathbf{w}})], & t \in (0, T] \\ \delta G = 0, & t = 0. \end{cases} \quad (4.3)$$

From (2.6), we have $U_C - \tilde{U}_C = \left(\mathbf{x} \cdot (\mathbf{u} - \tilde{\mathbf{u}}) + \sum_i \frac{x_i^2}{2} (v_i - \tilde{v}_i) \right)$, and from (2.8) we get $\Theta_{U_C - \tilde{U}_C}[G] = (\mathbf{u} - \tilde{\mathbf{u}}) \cdot \nabla_{\mathbf{p}} G + \sum_i x_i (v_i - \tilde{v}_i) \frac{\partial G}{\partial p_i}$. Now, we apply Theorem 3.1 to the problem (4.3), and obtain

$$\begin{aligned} \|\delta G(\cdot, \cdot, t)\|_{H_{k-1}^1} &\leq \left(\left\| \Theta_{U_C - \tilde{U}_C}[G(\tilde{\mathbf{u}})] \right\|_{L^1([0, T]; H_{k-1}^1)} \right) \times \\ &\quad \exp \left(C \left(\|\mathbf{u} + \mathbf{v}\|_{L^1([0, T])} + \|U_0\|_{L^1([0, T]; C_b^{2k-1})} + \frac{T}{2} \right) \right). \end{aligned} \quad (4.4)$$

We estimate the H_k^1 norm of the non-homogeneous term.

$$\begin{aligned} \left\| \Theta_{U_C - \tilde{U}_C}[G(\tilde{\mathbf{w}})] \right\|_{H_{k-1}^1}^2 &\leq |\mathbf{u} - \tilde{\mathbf{u}}|^2 \|\nabla_{\mathbf{p}} G(\tilde{\mathbf{w}})\|_{H_{k-1}^1}^2 + C |\mathbf{v} - \tilde{\mathbf{v}}|^2 \|\nabla_{\mathbf{p}} G(\tilde{\mathbf{w}})\|_{H_k^1}^2 \\ &\leq C \left(|\mathbf{u} - \tilde{\mathbf{u}}|^2 + |\mathbf{v} - \tilde{\mathbf{v}}|^2 \right) \|G(\tilde{\mathbf{w}})\|_{H_k^2}^2. \end{aligned}$$

We have used the estimate

$$\sum_i \left(x_i (v_i - \tilde{v}_i) \frac{\partial G}{\partial p_i} \right)^2 \leq |\mathbf{v} - \tilde{\mathbf{v}}|^2 (\nabla_{\mathbf{p}} G(\tilde{\mathbf{w}}))^2 (1 + |\mathbf{x}|)^2,$$

and $(1 + |\mathbf{x}|^k + |\mathbf{p}|^k)^2 (1 + |\mathbf{x}|)^2 \leq C (1 + |\mathbf{x}|^{k+1} + |\mathbf{p}|^{k+1})^2$, which follows easily from the Young's inequality $a^k \leq \frac{k}{k+1} a^{k+1} + k + 1$, where $a \leq 0$ and $k \in \mathbb{N}$.

Applying Theorem 3.2 to $G(\tilde{\mathbf{w}})$, we obtain

$$\begin{aligned} \|G(\tilde{\mathbf{w}})(\cdot, \cdot, t)\|_{H_k^2} &\leq \left(\|f_0\|_{H_k^2} + C \|g\|_{L^1([0, T]; H_k^2)} \right) \times \\ &\quad \exp \left(C \left(\|\tilde{\mathbf{u}} + \tilde{\mathbf{v}}\|_{L^1([0, T]; \ell_1^n)} + \|U_0\|_{L^1([0, T]; C_b^{2k+2})} + T \right) \right). \end{aligned}$$

Equation (4.4) gives

$$\begin{aligned} \|\delta G(\cdot, \cdot, t)\|_{H_{k-1}^1} &\leq C \int_0^t \left(|\mathbf{u} - \tilde{\mathbf{u}}|^2 + |\mathbf{v} - \tilde{\mathbf{v}}|^2 \right)^{\frac{1}{2}} dt \\ &\quad \left(\|f_0\|_{H_k^2} + C \|g\|_{L^1([0, T]; H_k^2)} \right) \times \\ &\quad \exp \left(C \left(\|\mathbf{u} + \mathbf{v}\|_{L^1([0, T]; \ell_1^n)} + \|U_0\|_{L^1([0, T]; C_b^{2k+2})} + T \right) \right). \end{aligned}$$

□

In the following lemma, we state that G , for fixed $f_0 \in H_k^m$, $m \in \{1, 2, 3\}$ and $k \in \mathbb{N}$, is weak-weak continuous from $\mathcal{U}$ into $L^\infty([0, T]; H_k^m)$. The proof of this lemma is standard and is omitted (see, e.g., [1]).

Lemma 4.2. *Under assumptions (A.1)-(A.2)-(A.3)-(A.4), let $\mathbf{w} \in \mathcal{U}$ and $(\mathbf{w}^l) \subset \mathcal{U}$ be a weakly convergent sequence of controls such that $\mathbf{w}^l \xrightarrow{*} \mathbf{w}$ in $L^\infty([0, T]; \mathbb{R}^{2n}) \cap \mathcal{U}$. Then $G(\mathbf{w}^l) \xrightarrow{*} G(\mathbf{w})$ in the weak-* topology of $L^\infty([0, T]; H_k^m)$.*

Next, we investigate the differentiability of the Wigner control-to-state map. We start considering the Gateaux derivative of this map. For this purpose, let $\mathbf{w}$ be an admissible control pair and define

$$\delta^\varepsilon G(\mathbf{w}; \delta \mathbf{w}) \doteq \frac{G(\mathbf{w} + \varepsilon \delta \mathbf{w}) - G(\mathbf{w})}{\varepsilon},$$

where $\delta \mathbf{w} \in L^1([0, T]; \mathbb{R}^{2n}) \cap L^\infty([0, T]; \mathbb{R}^{2n})$.

Then the Gateaux derivative of G at $\mathbf{w}$ in the direction $\delta \mathbf{w}$ is defined as the following limit

$$\delta^0 G(\mathbf{w}; \delta \mathbf{w}) \doteq \lim_{\varepsilon \rightarrow 0^+} \delta^\varepsilon G(\mathbf{w}; \delta \mathbf{w}). \quad (4.5)$$

Whenever possible, in the following we shall omit to write the arguments $(\mathbf{w}; \delta \mathbf{w})$. According to the previous discussion, $\delta^\varepsilon G$ is a solution to

$$\partial_t \delta^\varepsilon G + \mathbf{p} \cdot \nabla_{\mathbf{x}} \delta^\varepsilon G - \Theta_{U_0 + U_C(\mathbf{w})}[\delta^\varepsilon G] = \Theta_{U_C(\delta \mathbf{w})}[G(\mathbf{w} + \varepsilon \delta \mathbf{w})]. \quad (4.6)$$

Lemma 4.1 gives ($\varepsilon < 1$)

$$\|\delta^\varepsilon G(\cdot, \cdot, t)\|_{H_{k-1}^1} \leq K \int_0^t \left(|\delta \mathbf{u}|^2 + |\delta \mathbf{v}|^2 \right)^{\frac{1}{2}} dt, \quad (4.7)$$

where $K = K(\delta \mathbf{w}; f_0, g, U_0)$ is defined in (4.1).

Equation (4.7) provides a uniform bound of the $L^\infty([0, T]; H_{k-1}^1)$ norm of the sequence $\delta^\varepsilon G$. For small ε , possibly after the extraction of a subsequence, $\delta^\varepsilon G$ converges to some $\delta^0 G$ in the weak- $*$ topology (same arguments as in Prop. 3.3 of [1]). In order to obtain the equation satisfied by $\delta^0 G$, we write Eq. (4.6) in weak form

$$\begin{aligned} & - \int_0^T \int_{\mathbb{R}^{2n}} \left(\delta^\varepsilon G \partial_t \varphi + \mathbf{p} \cdot \delta^\varepsilon G \nabla_{\mathbf{x}} \varphi - \delta^\varepsilon G \Theta_{U_0 + U_C(\mathbf{w})}[\varphi] \right) d\mathbf{x} d\mathbf{p} dt \\ & = - \int_0^T \int_{\mathbb{R}^{2n}} G(\mathbf{w} + \varepsilon \delta \mathbf{w}) \Theta_{U_C(\delta \mathbf{w})}[\varphi] d\mathbf{x} d\mathbf{p} dt, \quad \forall \varphi \in \mathcal{D}, \end{aligned}$$

where $\mathcal{D}$ denotes the space of test functions. Taking the limit $\varepsilon \rightarrow 0$ (using $G(\mathbf{w} + \varepsilon \delta \mathbf{w}) \xrightarrow{s} G(\mathbf{w})$) we have that $\delta^0 G$ satisfies the following equation in weak form

$$\partial_t \delta^0 G + \mathbf{p} \cdot \nabla_{\mathbf{x}} \delta^0 G - \Theta_{U_0 + U_C(\mathbf{w})}[\delta^0 G] = \Theta_{U_C(\delta \mathbf{w})}[G(\mathbf{w})]. \quad (4.8)$$

We shall now verify that the convergence $\delta^\varepsilon G \rightarrow \delta^0 G$ is strong. We define $\rho^\varepsilon = \delta^\varepsilon G - \delta^0 G$ and take the difference between (4.6) and (4.8)

$$\begin{cases} \partial_t \rho^\varepsilon + \mathbf{p} \cdot \nabla_{\mathbf{x}} \rho^\varepsilon - \Theta_{U_0 + U_C(\mathbf{w})}[\rho^\varepsilon] = \varepsilon \Theta_{U_C(\delta \mathbf{w})}[\delta^\varepsilon G], \\ \rho^\varepsilon|_{t=0} = 0. \end{cases} \quad (4.9)$$

Application of Theorem 3.1 gives

$$\begin{aligned} \|\rho(\cdot, \cdot, t)\|_{H_k^1} &\leq \varepsilon C \int_0^t \left\| \Theta_{U_C(\delta \mathbf{w})}[\delta^\varepsilon G](\cdot, \cdot, \tau) \right\|_{H_k^1} d\tau \times \\ &\quad \exp \left(C \int_0^t \left(|\mathbf{u}(\tau)| + |\mathbf{v}(\tau)| + \|U_0(\tau)\|_{C_b^{2k+1}} \right) d\tau + C \frac{t}{2} \right), \end{aligned} \quad (4.10)$$

and, using (4.7), we obtain

$$\begin{aligned} \left\| \Theta_{U_C(\delta \mathbf{w})}[\delta^\varepsilon G] \right\|_{H_{k-1}^1} &\leq C \left(|\delta \mathbf{u}|^2 + |\delta \mathbf{v}|^2 \right)^{\frac{1}{2}} \|\delta^\varepsilon G\|_{H_k^2} \\ &\leq K \left(|\delta \mathbf{u}|^2 + |\delta \mathbf{v}|^2 \right)^{\frac{1}{2}} \int_0^t \left(|\delta \mathbf{u}|^2 + |\delta \mathbf{v}|^2 \right)^{\frac{1}{2}} dt, \end{aligned}$$

where $K = K(\delta u; f_0, g, U_0, d)$ defined in (4.1) and

$$\begin{aligned} \|\rho(\cdot, \cdot, t)\|_{H_k^1} &\leq \varepsilon C K \left(\int_0^t \left(|\delta \mathbf{u}|^2 + |\delta \mathbf{v}|^2 \right)^{\frac{1}{2}} d\tau \right)^2 \times \\ &\quad \exp \left(C \int_0^t \left(|\mathbf{u}(\tau)| + |\mathbf{v}(\tau)| + \|U_0(\tau)\|_{C_b^{2k+1}} \right) d\tau + C \frac{t}{2} \right). \end{aligned} \quad (4.11)$$

We obtain $\rho^\varepsilon \rightarrow 0$ in $L^\infty([0, T]; H_k^1)$, for $\varepsilon \rightarrow 0$. These preliminary estimates lead to the main result of this section:

Theorem 4.1. *The map G is Fréchet differentiable from $L^\infty([0, T]; \mathbb{R}^{2n})$ to $L^\infty([0, T]; H_k^1)$ for any $k \in \mathbb{N}$, and the Fréchet derivative $DG(U)$ agrees with the Gateaux derivative $\delta^0 G$.*

Proof: We consider

$$\mathcal{G}(\mathbf{w}, \delta \mathbf{w}) \doteq G(\mathbf{w} + \delta \mathbf{w}) - G(\mathbf{w}) - \delta^0 G(\mathbf{w}, \delta \mathbf{w}).$$

Using the same procedure as for Eq. (4.9), we obtain that $\mathcal{G}$ satisfies the problem

$$\begin{cases} \partial_t \mathcal{G} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \mathcal{G} - \Theta_{U_0 + U_C(\mathbf{w})}[\mathcal{G}] = \Theta_{U_C(\delta \mathbf{w})}[G(\mathbf{w} + \delta \mathbf{w}) - G(\mathbf{w})], \\ \mathcal{G}|_{t=0} = 0. \end{cases} \quad (4.12)$$

and we get an estimate analogous to Eq. (4.11)

$$\|\mathcal{G}\|_{L^\infty([0, T]; H_k^1)} \leq C' \left(\int_0^t \left(|\delta \mathbf{u}|^2 + |\delta \mathbf{v}|^2 \right)^{\frac{1}{2}} d\tau \right)^2. \quad (4.13)$$

This leads to

$$\lim_{\|\delta \mathbf{w}\|_{L^\infty([0, T]; \mathbb{R}^{2n})} \rightarrow 0} \frac{\|G(\mathbf{w} + \delta \mathbf{w}) - G(\mathbf{w}) - \delta^0 G(\mathbf{w}, \delta \mathbf{w})\|_{L^\infty([0, T]; H_k^1)}}{\|\delta \mathbf{w}\|_{L^\infty([0, T]; \mathbb{R}^{2n})}} = 0. \quad (4.14)$$

□

5 Ensemble optimal control problems

In this section, we formulate ensemble optimal control problems governed by the Wigner equation. As indicated in the Introduction, the purpose of the control is the minimisation of a cost functional. Since in many applications is of particular importance to minimize (or maximixize) the value of the observables at the final time $t = T$ and to steer the distribution function along a given path $(\mathbf{x}_t, \mathbf{p}_t)$, we consider the following functionals

$$\begin{aligned}\Phi(f) &= - \int_{\mathbb{R}^{2n}} A(\mathbf{x}, \mathbf{p}) f(\mathbf{x}, \mathbf{p}, T) \, d\mathbf{x} \, d\mathbf{p} \\ \Psi(f) &= \int_0^T \int_{\mathbb{R}^{2n}} V(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{p}, t) \, d\mathbf{x} \, d\mathbf{p} \, dt .\end{aligned}$$

The function V represents a phase space valley where f should concentrate, for example, $V(\mathbf{x}, \mathbf{p}) = -C e^{-[(\mathbf{x}-\mathbf{x}_t)^2 + (\mathbf{p}-\mathbf{p}_t)^2]}$. The functionals Φ and Ψ achieve the control on the final value of the observable A and the concentration of the distribution on the phase space, respectively.

In general, we assume that the functions A and V above are bounded. Therefore the functionals Φ and Ψ are linear and continuous in f and so weakly lower semi-continuous.

In addition to defining the purpose of the control, we need to measure the cost of its action that should be kept as small as possible. For this reason, we consider a cost term of the form

$$\kappa(\mathbf{w}) = \frac{1}{2} \int_0^T \left(\gamma(|\mathbf{u}(t)|^2 + |\mathbf{v}(t)|^2) + \nu \left(\left| \frac{d\mathbf{u}}{dt} \right|^2 + \left| \frac{d\mathbf{v}}{dt} \right|^2 \right) \right) dt, \quad (5.1)$$

where $\gamma, \nu > 0$, and the factor $1/2$ is chosen for convenience of later calculations. In (5.1), the first two terms can be interpreted as the energy of the control, whereas the other terms measure its variation in time. Notice that, by requiring $\nu > 0$, the control function $\mathbf{w}$ must be in $\mathcal{U}$ (recall definition (2.7)), since (5.1) represents a weighted $H^1(0, T)$ norm. Notice that $\kappa(\mathbf{w})$ is strictly convex in $\mathcal{U}$.

With this preparation, we can formulate our Wigner ensemble optimal control problem as follows:

$$\begin{aligned}\min J(f, \mathbf{w}) &:= \Phi(f) + \Psi(f) + \kappa(\mathbf{w}), \\ \text{s.t.} \quad \partial f + \mathbf{p} \cdot \nabla_{\mathbf{x}} f - \Theta_{U_0+U_C(\mathbf{w})}[f] &= 0, \\ f|_{t=0} &= f_0, \quad f_0 \in H_k^1 \\ \mathbf{w} &\in \mathcal{U}.\end{aligned} \quad (5.2)$$

Specifically, in (5.2) we have the following cost functional

$$J(f, \mathbf{w}) = \int_0^T \int_{\mathbb{R}^{2n}} V(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{p}, t) \, d\mathbf{x} \, d\mathbf{p} \, dt - \int_{\mathbb{R}^{2n}} A(\mathbf{x}, \mathbf{p}) f(\mathbf{x}, \mathbf{p}, T) \, d\mathbf{x} \, d\mathbf{p} + \kappa(\mathbf{w}) \quad (5.3)$$

Clearly, $J(f, \mathbf{w})$ is bounded from below and weakly lower semi-continuous.

According to Theorem 3.1, for every $\mathbf{w} \in \mathcal{U}$ and $k \in \mathbb{N}$, $f_0 \in H_k^1$, there exists a Wigner function $f = G(\mathbf{w}) \in C([0, T]; H_k^1)$ satisfying the constraints in (5.2) (i.e. the Cauchy problem for the Wigner equation). We recall that the control-to-state map G is continuous. Thus, we can introduce the following reduced cost functional

$$\hat{J}(\mathbf{w}) := J(G(\mathbf{w}), \mathbf{w}), \quad (5.4)$$

so that the optimal control problem (5.2) can be equivalently written as follows

$$\min_{\mathbf{w} \in \mathcal{U}} \hat{J}(\mathbf{w}). \quad (5.5)$$

Theorem 5.1. *Under assumptions (A.1)-(A.2)-(A.3)-(A.4), $f_0 \in H_k^1$, the ensemble optimal control problem (5.2) (resp. (5.5)) admits at least one solution $\mathbf{w}^* \in \mathcal{U}$. The corresponding state $f^* := G(\mathbf{w}^*)$ belongs to the space $C([0, T]; H_k^1)$.*

Proof. If $(f, \mathbf{w}) \in C([0, T]; H_k^1) \times H^1([0, T], \mathbb{R}^{2n})$, the functional J given in (5.3) is well-defined and coercive in $\mathbf{w} \in \mathcal{U}$. Furthermore, due to estimate (3.6) in Theorem 3.1, we have that the map G takes its values in a bounded set of $L^\infty([0, T], H_k^0)$. It follows that $\hat{J}$ is bounded. Moreover, since G is weak-weak continuous, as stated in Lemma 4.2, and J is weakly lower semi-continuous, we can state that $\hat{J}$ is weakly lower semi-continuous.

Therefore, if $(\mathbf{w}_n) \subset \mathcal{U}$ is a sequence which converges weakly to a $\mathbf{w} \in \mathcal{U}$, we have

$$\liminf_{n \rightarrow +\infty} \hat{J}(\mathbf{w}_n) = \liminf_{n \rightarrow +\infty} J(G(\mathbf{w}_n), \mathbf{w}_n) \geq J(G(\mathbf{w}), \mathbf{w}) = \hat{J}(\mathbf{w}).$$

With this preparation, the proof of existence of a minimizer for $\hat{J}$ is standard: take a minimizing sequence $(\mathbf{w}_n) \subset \mathcal{U}$, and recall the J is coercive in $\mathbf{w}$. Thus the sequence is bounded and we can extract a weakly convergent subsequence whose limit is $\mathbf{w}^* \in \mathcal{U}$. Then, by the weak lower semi-continuity of $\hat{J}$, we conclude that $\mathbf{w}^*$ is a minimizer for $\hat{J}$. $\square$

6 Optimality System

In optimal control theory with differential models, we have the task to characterize solutions to optimal control problems. However, in the case of nonlinear control mechanisms, as in our model, we can have many local and global minima. Thus, although the proof of existence by minimizing sequences (Theorem 5.1) refers to (possibly non unique) global minima for our ensemble control problem (5.2), the differential characterization by first-order optimality conditions (optimality system) applies in the same way to local and global minima, which include $\mathbf{w}^*$. We remark that the knowledge of the optimality system is crucial for the development of any gradient-based method for the numerical solution of optimal control problems; see, e.g., [9].

In order to derive the optimality system, we discuss Fréchet differentiability of $\hat{J}(\mathbf{w})$, and use a Lagrangian framework in order to derive the first-order optimality conditions.

Concerning the differentiability of the reduced cost functional, we have the following.

Theorem 6.1. *The map $\hat{J}(\mathbf{w})$ defined in Eq. (5.4) is Fréchet differentiable from $L^\infty([0, T]; \mathbb{R}^{2n}) \cap \mathcal{U}$ to $\mathbb{R}$.*

Proof: We set $\hat{J} = \hat{J}_1 - \hat{J}_2 + \kappa(\mathbf{w})$ where

$$\begin{aligned}\hat{J}_1 &= \Psi(G(\mathbf{w})) = \int_0^T \int_{\mathbb{R}^{2n}} G(\mathbf{w})(\mathbf{x}, \mathbf{p}, t) V(\mathbf{x}, \mathbf{p}, t) \, d\mathbf{x} \, d\mathbf{p} \, dt, \\ \hat{J}_2 &= -\Phi(G(\mathbf{w})) = \int_{\mathbb{R}^{2n}} G(\mathbf{w})(\mathbf{x}, \mathbf{p}, T) A(\mathbf{x}, \mathbf{p}) \, d\mathbf{x} \, d\mathbf{p}.\end{aligned}$$

We first consider the differentiability of $\hat{J}_1(\mathbf{w})$. We define

$$D\hat{J}_1(\mathbf{w}) \doteq \int_0^T \int_{\mathbb{R}^{2n}} \delta^0 G(\mathbf{w}) V(\mathbf{x}, \mathbf{p}, t) (\mathbf{x}, \mathbf{p}, t) \, d\mathbf{x} \, d\mathbf{p} \, dt,$$

where $\delta^0 G$ is defined in Eq. (4.5). Then, we have

$$\begin{aligned}& \left| \hat{J}_1(\mathbf{w} + \delta\mathbf{w}) - \hat{J}_1(\mathbf{w}) - D\hat{J}_1(\mathbf{w}) \right| \\ & \leq \int_0^T \int_{\mathbb{R}^{2n}} \left| G(\mathbf{w} + \delta\mathbf{w}) - G(\mathbf{w}) - \delta^0 G \right| |V| \, d\mathbf{x} \, d\mathbf{p} \, dt \\ & \leq C \int_0^T \int_{\mathbb{R}^{2n}} \left| G(\mathbf{w} + \delta\mathbf{w}) - G(\mathbf{w}) - \delta^0 G \right| \, d\mathbf{x} \, d\mathbf{p} \, dt,\end{aligned}$$

where $C = \|V\|_{L^\infty([0, T]; L^\infty(\mathbb{R}^{2n}))}$. The last integral can be estimated by Hölder inequality. For any $k \in \mathbb{N}$ such that $k > \frac{n}{2}$ we have (remind the definition $r^k \doteq |\mathbf{x}|^k + |\mathbf{p}|^k$):

$$\begin{aligned}\int_{\mathbb{R}^{2n}} \left| G(\mathbf{w} + \delta\mathbf{w}) - G(\mathbf{w}) - \delta^0 G \right| \, d\mathbf{x} \, d\mathbf{p} & \leq \left(\int_{\mathbb{R}^{2n}} \frac{1}{(1 + r^k)^2} \, d\mathbf{x} \, d\mathbf{p} \right)^{\frac{1}{2}} \\ & \times \left(\int_{\mathbb{R}^{2n}} \left| G(\mathbf{w} + \delta\mathbf{w}) - G(\mathbf{w}) - \delta^0 G \right|^2 (1 + r^k)^2 \, d\mathbf{x} \, d\mathbf{p} \right)^{\frac{1}{2}} \\ & \leq C \left\| G(\mathbf{w} + \delta\mathbf{w}) - G(\mathbf{w}) - \delta^0 G \right\|_{L_k^2}.\end{aligned}$$

In this way we have obtained

$$\begin{aligned}& \left| \hat{J}_1(\mathbf{w} + \delta\mathbf{w}) - \hat{J}_1(\mathbf{w}) - D\hat{J}_1(\mathbf{w}) \right| \\ & \leq C \int_0^T \left\| G(\mathbf{w} + \delta\mathbf{w}) - G(\mathbf{w}) - \delta^0 G \right\|_{L_k^2} \, dt \\ & \leq C \left\| G(\mathbf{w} + \delta\mathbf{w}) - G(\mathbf{w}) - \delta^0 G \right\|_{L^\infty([0, T]; L_k^2)}\end{aligned}$$

and we can evaluate the Fréchet derivative

$$\begin{aligned}& \lim_{\|\delta\mathbf{w}\|_{H^1([0, T]; \mathbb{R}^{2n})} \rightarrow 0} \frac{\left| \hat{J}_1(\mathbf{w} + \delta\mathbf{w}) - \hat{J}_1(\mathbf{w}) - D\hat{J}_1(\mathbf{w}) \right|}{\|\delta\mathbf{w}\|_{H^1([0, T]; \mathbb{R}^{2n})}} \\ & \leq C \lim_{\|\delta\mathbf{w}\|_{H^1([0, T]; \mathbb{R}^{2n})} \rightarrow 0} \frac{\left\| G(\mathbf{w} + \delta\mathbf{w}) - G(\mathbf{w}) - \delta^0 G \right\|_{L^\infty([0, T]; L_k^2)}}{\|\delta\mathbf{w}\|_{L^\infty([0, T]; \mathbb{R}^{2n})}} = 0,\end{aligned}$$

where we have used Eq. (4.14) and the estimate

$$\|\delta \mathbf{w}\|_{L^\infty([0,T];\mathbb{R}^{2n})} \leq C \|\delta \mathbf{w}\|_{H^1([0,T];\mathbb{R}^{2n})}.$$

The term $\hat{J}_2$ can be treated in the same way. The last term $\kappa(\mathbf{w})$ of $\hat{J}$ is easily seen to be Fréchet differentiable. $\square$

Since $\hat{J}(\mathbf{w})$ is Fréchet differentiable, we can characterize an optimal control as a solution to the first-order optimality condition given by

$$\nabla_{\mathbf{w}} \hat{J}(\mathbf{w}) = 0,$$

where $\nabla_{\mathbf{w}}$ denotes the Fréchet gradient in $\mathcal{U}$.

It is convenient to discuss this characterization by following Lagrange's approach, which formally requires to introduce the Lagrange functional

$$\mathcal{L}(f, \mathbf{w}, h) \doteq J(f, \mathbf{w}) + \int_0^T \int_{\mathbb{R}^{2n}} \left(\partial_t f + \mathbf{p} \cdot \nabla_{\mathbf{x}} f - \Theta_{U(\mathbf{w})}[f] \right) h(\mathbf{x}, \mathbf{p}, t) \, d\mathbf{x} \, d\mathbf{p} \, dt,$$

where h is the lagrangian multiplier. It follows from the results in the previous sections that this Lagrange functional is Fréchet differentiable and we actually computed the Gateaux derivatives. In this framework, the optimality system corresponds to requiring that the derivatives of $\mathcal{L}$ with respect to its arguments to f , $\mathbf{w}$ and h are zero. Notice that we assume that the initial condition f_0 is given.

We start by deriving $\mathcal{L}$ with respect to h . We have

$$(\nabla_h \mathcal{L}, \delta h) = \int_0^T \int_{\mathbb{R}^{2n}} \left(\partial_t f + \mathbf{p} \cdot \nabla_{\mathbf{x}} f - \Theta_{U(\mathbf{w})}[f] \right) \delta h \, d\mathbf{x} \, d\mathbf{p} \, dt.$$

Hence, $(\nabla_h \mathcal{L}, \delta h) = 0$ corresponds to the weak formulation of the Wigner equation.

Next, we derive $\mathcal{L}$ with respect to f , obtaining

$$\begin{aligned} (\nabla_f \mathcal{L}, \delta f) &= \int_0^T \int_{\mathbb{R}^{2n}} \left(V - \partial_t h - \mathbf{p} \cdot \nabla_{\mathbf{x}} h + \Theta_{U(\mathbf{w})}[h] \right) \delta f \, d\mathbf{x} \, d\mathbf{p} \, dt \\ &\quad + \int_{\mathbb{R}^{2n}} [h(\mathbf{x}, \mathbf{p}, T) - A(\mathbf{x}, \mathbf{p})] \delta f(\mathbf{x}, \mathbf{p}, T) \, d\mathbf{x} \, d\mathbf{p}, \end{aligned}$$

where $\delta f(\mathbf{x}, \mathbf{p}, 0) = 0$ and we used an integration by parts. Therefore, by requiring $\nabla_f \mathcal{L}(f, \mathbf{w}, h) = 0$, we obtain the adjoint problem

$$\begin{cases} \partial_t h + \mathbf{p} \cdot \nabla_{\mathbf{x}} h - \Theta_{U(\mathbf{w})}[h] = V, & \text{in } \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n \times [0, T] \\ h|_{t=T} = A, & \text{on } \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n \end{cases}, \quad (6.1)$$

where $h(\mathbf{x}, \mathbf{p}, T) = A(\mathbf{x}, \mathbf{p})$ is the terminal condition.

We remark that this adjoint problem has the same structure of the nonhomogeneous Wigner problem (3.1) with g replaced by V and f_0 replaced by A . Therefore, assuming

that V and A satisfy the assumptions (A.3) and (A.4), respectively, our results for the Wigner problem are also valid for the adjoint problem.

Next, we focus on the derivative of the Lagrangian with respect to the control functions. In this case, the calculation of the Gateaux derivative reveals an additional modelling issue, that is, the choice of appropriate initial and terminal conditions for $\mathbf{u}$ and $\mathbf{v}$. In particular, we can require that the controls are switched on at $t = 0$ and switched off at $t = T$, which means $\mathbf{w}(0) = 0$ and $\mathbf{w}(T) = 0$. Subject to this assumption, we have

$$\begin{aligned} (\nabla_{\mathbf{u}}\mathcal{L}(f, \mathbf{w}, h), \delta\mathbf{u}) &= (\nabla_{\mathbf{u}}J(f, \mathbf{w}), \delta\mathbf{u}) \\ &+ \lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\mathbb{R}^{2n}} \frac{\Theta_{UC}(\mathbf{w} + \varepsilon\delta\mathbf{u})[f] - \Theta_{UC}(\mathbf{w})[f]}{\varepsilon} h \, d\mathbf{x} \, d\mathbf{p} \, dt \\ &= (\nabla_{\mathbf{u}}J(f, \mathbf{w}), \delta\mathbf{u}) + \int_0^T \int_{\mathbb{R}^{2n}} \Theta_{UC}(\delta\mathbf{u})[f] h \, d\mathbf{x} \, d\mathbf{p} \, dt, \end{aligned}$$

and, similarly,

$$(\nabla_{\mathbf{v}}\mathcal{L}(f, \mathbf{w}, h), \delta\mathbf{v}) = (\nabla_{\mathbf{v}}J(f, \mathbf{w}), \delta\mathbf{v}) + \int_0^T \int_{\mathbb{R}^{2n}} \Theta_{UC}(\delta\mathbf{v})[f] h \, d\mathbf{x} \, d\mathbf{p} \, dt.$$

First, we evaluate

$$\begin{aligned} (\nabla_{\mathbf{u}}J(f, \mathbf{w}), \delta\mathbf{u}) &= \\ \lim_{\varepsilon \rightarrow 0} \frac{1}{2\varepsilon} \int_0^T &\left(\gamma \left(|\mathbf{u} + \varepsilon\delta\mathbf{u}|^2 - |\mathbf{u}|^2 \right) + \nu \left(\left| \frac{d\mathbf{u} + \varepsilon d\delta\mathbf{u}}{dt} \right|^2 - \left| \frac{d\mathbf{u}}{dt} \right|^2 \right) \right) dt \\ &= \int_0^T \left(\gamma (\mathbf{u} \cdot \delta\mathbf{u}) + \nu \frac{d(\mathbf{u} \cdot \delta\mathbf{u})}{dt} \right) dt = \int_0^T \left(\gamma \mathbf{u} - \nu \frac{d^2(\mathbf{u})}{dt^2} \right) \cdot \delta\mathbf{u} \, dt, \end{aligned}$$

and the analogous for $(\nabla_{\mathbf{v}}J(f, \mathbf{w}), \delta\mathbf{v})$. Moreover, we have

$$\Theta_{UC}(\delta\mathbf{w})[f] = \delta\mathbf{u} \cdot \nabla_{\mathbf{p}}f + \sum_i \delta v_i \frac{x_i}{2} \frac{\partial f}{\partial p_i} = \left(\delta\mathbf{u} + \frac{1}{2} \delta\mathbf{v} \circ \mathbf{x} \right) \cdot \nabla_{\mathbf{p}}f,$$

and we obtain

$$\begin{aligned} &(\nabla_{\mathbf{u}}\mathcal{L}(f, \mathbf{w}, h), \delta\mathbf{u}) + (\nabla_{\mathbf{v}}\mathcal{L}(f, \mathbf{w}, h), \delta\mathbf{v}) \\ &= \int_0^T \left(\gamma \mathbf{u} - \nu \frac{d^2(\mathbf{u})}{dt^2} \right) \cdot \delta\mathbf{u} \, dt + \int_0^T \left(\gamma \mathbf{v} - \nu \frac{d^2(\mathbf{v})}{dt^2} \right) \cdot \delta\mathbf{v} \, dt \\ &\quad - \int_0^T \int_{\mathbb{R}^{2n}} h(\mathbf{x}, \mathbf{p}, t) \left(\delta\mathbf{u} + \frac{1}{2} \delta\mathbf{v} \circ \mathbf{x} \right) \cdot \nabla_{\mathbf{p}}f(\mathbf{x}, \mathbf{p}, t) \, d\mathbf{x} \, d\mathbf{p} \, dt. \end{aligned}$$

Now, requiring that $(\nabla_{\mathbf{w}}\mathcal{L}(f, \mathbf{w}, h), \delta\mathbf{w}) = 0$, we obtain the optimality condition equation

$$\begin{cases} \gamma u_i - \nu \frac{d^2 u_i}{dt^2} - \int_{\mathbb{R}^{2n}} h \frac{\partial f}{\partial p_i} \, d\mathbf{x} \, d\mathbf{p} = 0, & i = 1, \dots, n, \\ \gamma v_i - \nu \frac{d^2 v_i}{dt^2} - \int_{\mathbb{R}^{2n}} h \frac{x_i}{2} \frac{\partial f}{\partial p_i} \, d\mathbf{x} \, d\mathbf{p} = 0, & i = 1, \dots, n. \end{cases} \quad (6.2)$$

This problem is complemented with homogeneous initial and terminal conditions of Dirichlet type as discussed above.

Summarizing, the resulting optimality system consists of the forward Wigner problem (2.2), the adjoint problem (6.1), and the optimality condition (6.2).

$$\left\{ \begin{array}{ll} \frac{\partial f}{\partial t} + \mathbf{p} \cdot \nabla_{\mathbf{x}} f - \Theta_{U_0+U_C}[f] = 0, & \text{in } [0, T] \times \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n, \\ \frac{\partial h}{\partial t} + \mathbf{p} \cdot \nabla_{\mathbf{x}} h - \Theta_{U_0+U_C}[h] = V, & \text{in } [0, T] \times \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n, \\ f|_{t=0} = f_0, & \text{on } \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n, \\ h|_{t=T} = A, & \text{on } \mathbb{R}_{\mathbf{x}}^n \times \mathbb{R}_{\mathbf{p}}^n, \\ \gamma u_i - \nu \frac{d^2 u_i}{dt^2} - \int_{\mathbb{R}^{2n}} h \frac{\partial f}{\partial p_i} d\mathbf{x} d\mathbf{p} = 0, & i = 1, \dots, n, \\ \gamma v_i - \nu \frac{d^2 v_i}{dt^2} - \int_{\mathbb{R}^{2n}} h \frac{x_i}{2} \frac{\partial f}{\partial p_i} d\mathbf{x} d\mathbf{p} = 0, & i = 1, \dots, n. \end{array} \right. \quad (6.3)$$

where the control potential has the form given by Eq. (2.6).

7 Conclusion

An ensemble optimal control problem governed by the Wigner equation was formulated. This equation plays a central role in the statistical description of quantum systems in phase-space, which motivates the choice of ensemble cost functionals and of control mechanisms acting on the mean and variance of the Wigner density. These choices together with the presence of a pseudo-differential operator in the Wigner equation make this work unique in the field of quantum optimal control problems.

A detailed analysis in weighted Sobolev spaces of the proposed controlled Wigner model and of the corresponding optimization adjoint was presented. This analysis was further extended to prove existence of optimal controls and differentiability of the control-to-state map and of the ensemble cost functional, thus allowing the derivation of the optimality system that characterizes optimal controls.

This work should motivate further research in the field of optimal control problems governed by the Wigner equation. In fact, it would be possible to consider other control mechanisms as, e.g., boundary control problems. Moreover, the proposed ensemble control framework could be extended in order to accommodate other approaches for the manipulation of the Wigner function as in [38]. On the other hand, additional analysis is also required to further develop the present setting in order to include, e.g., constraints on the controls and semi-smooth costs, and to investigate second-order optimality conditions as in [23].

A Appendix

In this section we give the proofs of Lemma 3.1 and Theorem 3.2

Proof of Lemma 3.1

Proof: We multiply the Wigner equation (3.1) by $|\mathbf{x}|^k$ and we integrate with respect to the space and momentum coordinates. We obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \left\| |\mathbf{x}|^k f \right\|_{L^2}^2 &= \int_{\mathbb{R}^{2n}} \frac{\partial \left(|\mathbf{x}|^k f \right)}{\partial t} f |\mathbf{x}|^k d\mathbf{x} d\mathbf{p} \\ &= \underbrace{\frac{1}{2} \int_{\mathbb{R}^{2n}} f^2 \mathbf{p} \cdot \nabla_{\mathbf{x}} \left(|\mathbf{x}|^{2k} \right) d\mathbf{x} d\mathbf{p}}_{\doteq A_1} + \underbrace{\int_{\mathbb{R}^{2n}} |\mathbf{x}|^{2k} f \Theta_{U_0+U_C}[f] d\mathbf{x} d\mathbf{p}}_{\doteq A_2} \\ &\quad + \underbrace{\int_{\mathbb{R}^{2n}} |\mathbf{x}|^{2k} f g d\mathbf{x} d\mathbf{p}}_{\doteq A_3} . \end{aligned}$$

We use $\left| \mathbf{p} \cdot \nabla_{\mathbf{x}} \left(|\mathbf{x}|^{2k} \right) \right| \leq k \left(|\mathbf{x}|^2 + |\mathbf{p}|^2 \right)^k$, so that

$$|A_1| \leq \frac{k}{2} \int_{\mathbb{R}^{2n}} \left(|\mathbf{x}|^2 + |\mathbf{p}|^2 \right)^k f^2 d\mathbf{x} d\mathbf{p} .$$

The contribution to the term A_2 given by the control potential vanishes:

$$\int_{\mathbb{R}^{2n}} |\mathbf{x}|^{2k} f \Theta_{U_C}[f] d\mathbf{x} d\mathbf{p} = \frac{1}{2} \int_{\mathbb{R}^{2n}} |\mathbf{x}|^{2k} \left(\mathbf{u}(t) \cdot \nabla_{\mathbf{p}} f^2 + \sum_i x_i v_i(t) \frac{\partial f^2}{\partial p_i} \right) d\mathbf{x} d\mathbf{p} = 0 .$$

Then, we have

$$\begin{aligned} |A_2| &= \left| \int_{\mathbb{R}^{2n}} |\mathbf{x}|^{2k} f \Theta_{U_0}[f] d\mathbf{p} d\mathbf{x} \right| \\ &\leq \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} |\mathbf{x}|^{2k} |\delta U_0(\mathbf{x}, \boldsymbol{\eta}, t)| \left| \widehat{f}(\mathbf{x}, \boldsymbol{\eta}, t) \right|^2 d\boldsymbol{\eta} d\mathbf{x} \\ &\leq \frac{2}{\hbar} \|U_0\|_{L^\infty(\mathbb{R}_{\mathbf{x}}^n)} \int_{\mathbb{R}^n} |\mathbf{x}|^{2k} |f(\mathbf{x}, \mathbf{p}, t)|^2 d\mathbf{p} d\mathbf{x} , \end{aligned}$$

where we have used

$$\int_{\mathbb{R}^n} f \Theta_{U_0}[f](\mathbf{x}, \mathbf{p}, t) d\mathbf{p} = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \delta U_0(\mathbf{x}, \boldsymbol{\eta}, t) \left| \widehat{f}(\mathbf{x}, \boldsymbol{\eta}, t) \right|^2 d\boldsymbol{\eta} .$$

We have therefore obtained

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \left\| |\mathbf{x}|^k f \right\|_{L^2}^2 &\leq \frac{k}{2} \int_{\mathbb{R}^{2n}} \left(|\mathbf{x}|^2 + |\mathbf{p}|^2 \right)^k f^2 d\mathbf{x} d\mathbf{p} \\ &\quad + \frac{2}{\hbar} \|U_0\|_{L^\infty(\mathbb{R}_{\mathbf{x}}^n)} \int_{\mathbb{R}^n} |\mathbf{x}|^{2k} f^2 d\mathbf{p} d\mathbf{x} \\ &\quad + \int_{\mathbb{R}^{2n}} |\mathbf{x}|^{2k} |f g| d\mathbf{x} d\mathbf{p} . \end{aligned} \tag{A.1}$$

In a similar way, we multiply the Wigner equation (3.1) by $|\mathbf{p}|^k$ and integrate

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \left\| |\mathbf{p}|^k f \right\|_{L^2}^2 &= - \underbrace{\frac{1}{2} \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} \mathbf{p} \cdot \nabla_{\mathbf{x}} (f^2) \, d\mathbf{x} \, d\mathbf{p}}_{=0} \\ &\quad + \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} f \Theta_{U_0+U_C} [f] \, d\mathbf{x} \, d\mathbf{p} \\ &\quad + \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} g f \, d\mathbf{x} \, d\mathbf{p} . \end{aligned} \tag{A.2}$$

We can write

$$\begin{aligned} \left| \frac{1}{2} \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} (\mathbf{u} \cdot \nabla_{\mathbf{p}} f^2) \, d\mathbf{p} \right| &= \left| k \sum_i^n u_i \int_{\mathbb{R}^{2n}} p_i |\mathbf{p}|^{2(k-1)} f^2 \, d\mathbf{p} \right| \\ &\leq k \sum_i^n |u_i| \int_{\mathbb{R}^{2n}} |p_i| |\mathbf{p}|^{2(k-1)} f^2 \, d\mathbf{x} \, d\mathbf{p} \\ &\leq k \sum_i^n |u_i| \int_{\mathbb{R}^{2n}} \frac{1 + |\mathbf{p}|^2}{2} |\mathbf{p}|^{2(k-1)} f^2 \, d\mathbf{x} \, d\mathbf{p} \\ &\leq \frac{k}{2} \sum_i^n |u_i| \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^2)^k f^2 \, d\mathbf{x} \, d\mathbf{p} . \end{aligned} \tag{A.3}$$

and

$$\begin{aligned} \frac{1}{2} \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} \left(\sum_i^n x_i v_i \frac{\partial f^2}{\partial p_i} \right) \, d\mathbf{x} \, d\mathbf{p} \\ \leq \left(\sum_i^n |v_i| \right) \frac{k}{2} \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^2 + |\mathbf{x}|^2)^k f^2 \, d\mathbf{x} \, d\mathbf{p} . \end{aligned} \tag{A.4}$$

Using (A.3) and (A.4) in (A.2), we obtain for the control potential

$$\begin{aligned} \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} f \Theta_{U_C} [f] \, d\mathbf{x} \, d\mathbf{p} &\leq \frac{k}{2} \sum_i^n |u_i| \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^2)^k f^2 \, d\mathbf{x} \, d\mathbf{p} \\ &\quad + \left(\sum_i^n |v_i| \right) \frac{k}{2} \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^2 + |\mathbf{x}|^2)^k f^2 \, d\mathbf{x} \, d\mathbf{p} . \end{aligned}$$

Finally, we consider the confining potential U_0 . By using

$$\begin{aligned}
& (2\pi)^n \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} f \Theta_{U_0}[f] \, d\mathbf{x} \, d\mathbf{p} \\
&= \int_{\mathbb{R}^{4n}} f(\mathbf{x}, \mathbf{p}) f(\mathbf{x}, \mathbf{p}') \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \left(\sum_j^n -\frac{\partial^2}{\partial \eta_j^2} \right)^k e^{-i(\mathbf{p}-\mathbf{p}') \cdot \boldsymbol{\eta}} \, d\mathbf{p}' \, d\boldsymbol{\eta} \, d\mathbf{x} \, d\mathbf{p} \\
&= \int_{\mathbb{R}^{4n}} f(\mathbf{x}, \mathbf{p}) \overline{\widehat{f}(\mathbf{x}, \boldsymbol{\eta})} \left[\left(\sum_j^n -\frac{\partial^2}{\partial \eta_j^2} \right)^k \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \right] e^{-i\mathbf{p} \cdot \boldsymbol{\eta}} \, d\boldsymbol{\eta} \, d\mathbf{x} \, d\mathbf{p} \\
&= \left(\frac{\hbar^2}{2} \right)^k \int_{\mathbb{R}^{2n}} |\widehat{f}(\mathbf{x}, \boldsymbol{\eta})|^2 \left(\sum_j^n -\frac{\partial^2}{\partial x_j^2} \right)^k \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \, d\boldsymbol{\eta} \, d\mathbf{x},
\end{aligned}$$

we can estimate

$$\begin{aligned}
& \left| \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} f \Theta_{U_0}[f] \, d\mathbf{x} \, d\mathbf{p} \right| \\
& \leq \frac{2}{\hbar} \|U_0\|_{C_b^{2k}} \frac{1}{(2\pi)^n} \left(\frac{\hbar^2}{2} \right)^k \int_{\mathbb{R}^{2n}} |\widehat{f}(\mathbf{x}, \boldsymbol{\eta})|^2 \, d\boldsymbol{\eta} \, d\mathbf{x} \\
& = \frac{2}{\hbar} \left(\frac{\hbar^2}{2} \right)^k \|U_0\|_{C_b^{2k}} \|f\|_{L^2}^2.
\end{aligned}$$

We obtain

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} \left\| |\mathbf{p}|^k f \right\|_{L^2}^2 \\
& \leq \frac{k}{2} \sum_i^n (|u_i| + |v_i|) \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^2 + |\mathbf{x}|^2)^k f^2 \, d\mathbf{x} \, d\mathbf{p} \\
& \quad + \frac{2}{\hbar} \left(\frac{\hbar^2}{2} \right)^k \|U_0\|_{C_b^{2k}} \|f\|_{L^2}^2 + \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} |fg| \, d\mathbf{x} \, d\mathbf{p}.
\end{aligned} \tag{A.5}$$

Summing up (A.5), (A.1) and (A.1) for $k = 0$, we obtain

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^{2k} + |\mathbf{x}|^{2k}) f^2 \, d\mathbf{x} \, d\mathbf{p} \\
& \leq \frac{k}{2} \left(1 + \sum_i^n (|u_{1,i}| + |u_{2,i}|) \right) \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^{2k} + |\mathbf{x}|^{2k}) f^2 \, d\mathbf{x} \, d\mathbf{p} \\
& \quad + \|U_0\|_{C_b^{2k}} \frac{2}{\hbar} \left(1 + \left(\frac{\hbar^2}{2} \right)^k \right) \int_{\mathbb{R}^{2n}} (1 + |\mathbf{x}|^{2k}) f^2 \, d\mathbf{x} \, d\mathbf{p} \\
& \quad + \int_{\mathbb{R}^{2n}} (1 + |\mathbf{p}|^{2k} + |\mathbf{x}|^{2k}) |fg| \, d\mathbf{x} \, d\mathbf{p}.
\end{aligned}$$

For the last term, we use Hölder inequality

$$\begin{aligned} \int_{\mathbb{R}^{2n}} \left(1 + |\mathbf{p}|^{2k} + |\mathbf{x}|^{2k}\right) |fg| \, d\mathbf{x} \, d\mathbf{p} &\leq \\ \int_{\mathbb{R}^{2n}} \left(1 + |\mathbf{p}|^k + |\mathbf{x}|^k\right)^2 |fg| \, d\mathbf{x} \, d\mathbf{p} &\leq \|g\|_{L_k^2} \|f\|_{L_k^2} . \end{aligned}$$

Then, using the inequality

$$(1 + |\mathbf{x}|^{2k} + |\mathbf{p}|^{2k}) \geq \frac{1}{3} (1 + |\mathbf{x}|^k + |\mathbf{p}|^k)^2, \quad (\text{A.6})$$

we get

$$\frac{1}{2} \frac{d}{dt} \|f\|_{L_k^2}^2 \leq K \|f\|_{L_k^2}^2 + 3 \|g\|_{L_k^2} \|f\|_{L_k^2} ,$$

where

$$K = \frac{3k}{2} \left(1 + \sum_i^n (|u_i| + |v_i|)\right) + \|U_0\|_{C_b^{2k}} \frac{6}{\hbar} \left(1 + \left(\frac{\hbar^2}{2}\right)^k\right) .$$

In conclusion, we obtain

$$\frac{d}{dt} \|f\|_{L_k^2} \leq K \|f\|_{L_k^2} + 3 \|g\|_{L_k^2} , \quad (\text{A.7})$$

which proves Lemma 3.1 by applying the Grönwall lemma. $\square$

Proof of Theorem 3.2

Proof: In order to discuss the case of the H_k^2 norm, we denote by $\partial^2 f$ a generic second-order derivative of the Wigner function f with respect to space and momentum variables, namely

$$\partial^2 f \doteq \nabla_{\mathbf{p}}^\alpha \nabla_{\mathbf{x}}^\beta f$$

where (α, β) is a given couple of multi-indices with $|\alpha| + |\beta| = 2$.

We take the derivative of the Wigner equation

$$\partial_t(\partial^2 f) = -\mathbf{p} \cdot \nabla_{\mathbf{x}} \partial^2 f - \left(\partial^2 \mathbf{p}\right) \cdot \nabla_{\mathbf{x}} f + \partial^2 \Theta_{U_0+U_C}[f] + \partial^2 g .$$

By defining $r^k \doteq |\mathbf{x}|^k + |\mathbf{p}|^k$, we have

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\partial^2 f\|_{L^2}^2 &= \int_{\mathbb{R}^{2n}} \left[\frac{\mathbf{p}}{2} \cdot \left(\nabla_{\mathbf{x}} r^{2k}\right) \left(\partial^2 f\right)^2 + \left(1 + r^{2k}\right) \left(\partial^2 f\right) \partial^2 \Theta_{U_0+U_C}[f] \right. \\ &\quad \left. + \left(1 + r^{2k}\right) \left(\partial^2 f\right) \left(\partial^2 g\right) \right] d\mathbf{p} \, d\mathbf{x} \end{aligned} \quad (\text{A.8})$$

where we used $\partial^2 \mathbf{p} = 0$. The first term at the right-hand side of (A.8) is such that

$$\begin{aligned} \left| \int_{\mathbb{R}^{2n}} \frac{\mathbf{p}}{2} \cdot (\nabla_{\mathbf{x}} r^{2k}) (\partial^2 f)^2 \, d\mathbf{p} \, d\mathbf{x} \right| &= \left| \int_{\mathbb{R}^{2n}} \mathbf{p} \cdot \mathbf{x} k |\mathbf{x}|^{2(k-1)} (\partial^2 f)^2 \, d\mathbf{p} \, d\mathbf{x} \right| \\ &\leq C \int_{\mathbb{R}^{2n}} (1 + r^k)^2 (\partial^2 f)^2 \, d\mathbf{p} \, d\mathbf{x} . \end{aligned}$$

Regarding the second term, containing the potential U , we consider separately the one containing the confining potential U_0 and the one containing the control potential U_C . We start by writing

$$\begin{aligned} &\int_{\mathbb{R}^{2n}} (1 + r^{2k}) (\partial^2 f) \partial^2 \Theta_{U_0}[f] \, d\mathbf{x} \, d\mathbf{p} \\ &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{3n}} (1 + r^{2k}) (\partial^2 f(\mathbf{x}, \mathbf{p})) \partial^2 \left(\widehat{f(\mathbf{x}, \boldsymbol{\eta})} \delta U_0(\mathbf{x}, \boldsymbol{\eta}) e^{-i\mathbf{p} \cdot \boldsymbol{\eta}} \right) \, d\boldsymbol{\eta} \, d\mathbf{x} \, d\mathbf{p} . \end{aligned}$$

We write $|\mathbf{p}|^{2k}$ as follows

$$|\mathbf{p}|^{2k} = \left(\sum_i^n p_i^2 \right)^k = \sum_{|q|=k} \binom{k}{q} p^{2q} \equiv \sum_{|q|=k} \binom{k}{q} \prod_{i=1}^n p_i^{2q_i} .$$

We consider

$$\begin{aligned} I &\doteq (2\pi)^n \int_{\mathbb{R}^{2n}} |\mathbf{p}|^{2k} (\partial^2 f) \partial^2 \Theta_{U_0}[f] \, d\mathbf{x} \, d\mathbf{p} \\ &= \sum_{|q|=k} \binom{k}{q} \int_{\mathbb{R}^{2n}} \overline{\mathcal{F}_{\mathbf{p} \rightarrow \boldsymbol{\eta}} \left(p^q (\nabla_{\mathbf{x}}^\beta \nabla_{\mathbf{p}}^\alpha f) \right)} \mathcal{F}_{\mathbf{p} \rightarrow \boldsymbol{\eta}} \left(p^q \nabla_{\mathbf{x}}^\beta \nabla_{\mathbf{p}}^\alpha \Theta_{U_0}[f] \right) \, d\mathbf{x} \, d\boldsymbol{\eta} . \end{aligned}$$

We have

$$\begin{aligned} \overline{\mathcal{F}_{\mathbf{p} \rightarrow \boldsymbol{\eta}} \left(p^q \nabla_{\mathbf{x}}^\beta \nabla_{\mathbf{p}}^\alpha f \right)} &= (i)^q (-i)^\alpha \nabla_{\mathbf{x}}^\beta \nabla_{\boldsymbol{\eta}}^q \left(\boldsymbol{\eta}^\alpha \widehat{f(\mathbf{x}, \boldsymbol{\eta})} \right) \\ \mathcal{F}_{\mathbf{p} \rightarrow \boldsymbol{\eta}} \left(p^q \nabla_{\mathbf{x}}^\beta \nabla_{\mathbf{p}}^\alpha \Theta_{U_0}[f] \right) &= (-i)^q (i)^\alpha \nabla_{\mathbf{x}}^\beta \nabla_{\boldsymbol{\eta}}^q \left(\boldsymbol{\eta}^\alpha \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \widehat{f(\mathbf{x}, \boldsymbol{\eta})} \right) . \end{aligned}$$

We write

$$\begin{aligned} \nabla_{\mathbf{x}}^\beta \nabla_{\boldsymbol{\eta}}^q \left(\delta U_0(\mathbf{x}, \boldsymbol{\eta}) \boldsymbol{\eta}^\alpha \widehat{f(\mathbf{x}, \boldsymbol{\eta})} \right) &= \nabla_{\mathbf{x}}^\beta \sum_{s \leq q} \binom{q}{s} \left(\nabla_{\boldsymbol{\eta}}^{q-s} \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \right) \nabla_{\boldsymbol{\eta}}^s \left(\boldsymbol{\eta}^\alpha \widehat{f(\mathbf{x}, \boldsymbol{\eta})} \right) \\ &= \sum_{l \leq \beta} \sum_{s \leq q} \binom{\beta}{l} \binom{q}{s} \left(\nabla_{\mathbf{x}}^{\beta-l} \nabla_{\boldsymbol{\eta}}^{q-s} \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \right) \left(\nabla_{\mathbf{x}}^l \nabla_{\boldsymbol{\eta}}^s \boldsymbol{\eta}^\alpha \widehat{f(\mathbf{x}, \boldsymbol{\eta})} \right) , \end{aligned}$$

and we obtain

$$\begin{aligned} I &= \sum_{|q|=k} \binom{k}{q} \sum_{l \leq \beta; s \leq q} \binom{\beta}{l} \binom{q}{s} \times \\ &\int_{\mathbb{R}^{2n}} \left(\nabla_{\mathbf{x}}^\beta \nabla_{\boldsymbol{\eta}}^q \boldsymbol{\eta}^\alpha \widehat{f(\mathbf{x}, \boldsymbol{\eta})} \right) \left(\nabla_{\mathbf{x}}^{\beta-l} \nabla_{\boldsymbol{\eta}}^{q-s} \delta U_0(\mathbf{x}, \boldsymbol{\eta}) \right) \left(\nabla_{\mathbf{x}}^l \nabla_{\boldsymbol{\eta}}^s \boldsymbol{\eta}^\alpha \widehat{f(\mathbf{x}, \boldsymbol{\eta})} \right) \, d\mathbf{x} \, d\boldsymbol{\eta} . \end{aligned}$$

We estimate

$$\begin{aligned} |I| &\leq C \sum_q \sum_{l \leq \beta; s \leq q}^{|q|=k} \left\| \nabla_{\mathbf{x}}^{\beta-l} \nabla_{\boldsymbol{\eta}}^{q-s} \delta U_0 \right\|_{L^\infty(\mathbb{R}^{2n})} \int_{\mathbb{R}^{2n}} \left| \nabla_{\mathbf{x}}^\beta \nabla_{\boldsymbol{\eta}}^q \boldsymbol{\eta}^\alpha \widehat{f} \right| \left| \nabla_{\mathbf{x}}^l \nabla_{\boldsymbol{\eta}}^s \boldsymbol{\eta}^\alpha \widehat{f} \right| d\mathbf{x} d\boldsymbol{\eta} \\ &\leq C \|U\|_{C_b^{k+2}} \|f\|_{H_k^2}^2. \end{aligned}$$

The term obtained by multiplying $|\mathbf{x}|^{2k}$ instead of $|\mathbf{p}|^{2k}$ can be estimated similarly and we obtain

$$\left| \int_{\mathbb{R}^{2n}} (1 + |\mathbf{r}|^{2k}) (\partial^2 f) \partial^2 \Theta_{U_0}[f] d\mathbf{x} d\mathbf{p} \right| \leq C \|U_0\|_{C_b^{2k+2}} \|f\|_{H_k^2}^2.$$

Finally, we consider the term of Eq. (A.8) containing the control potential. Equation (2.8) gives

$$\partial^2 \Theta_{U_C}[f] = \mathbf{u} \cdot \nabla_{\mathbf{p}} \partial^2 f + \sum_i x_i v_i \frac{\partial \partial^2 f}{\partial p_i} + \sum_{i,j} v_i \left(\frac{\partial}{\partial p_j} \frac{\partial f}{\partial p_i} + \frac{\partial}{\partial x_j} \frac{\partial f}{\partial p_i} \right),$$

and

$$\begin{aligned} &\int_{\mathbb{R}^{2n}} (1 + r^{2k}) (\partial^2 f) \partial^2 \Theta_{U_C}[f] d\mathbf{x} d\mathbf{p} \\ &= \sum_{i,j} v_i \int_{\mathbb{R}^{2n}} (1 + r^{2k}) \left((\partial^2 f) \left(\frac{\partial}{\partial p_j} \frac{\partial f}{\partial p_i} + \frac{\partial}{\partial x_j} \frac{\partial f}{\partial p_i} \right) \right) d\mathbf{x} d\mathbf{p}. \end{aligned}$$

We obtain

$$\left| \int_{\mathbb{R}^{2n}} (1 + r^{2k}) (\partial^2 f) \partial^2 \Theta_{U_C}[f] d\mathbf{x} d\mathbf{p} \right| \leq C |\mathbf{v}| \|U_0\|_{C_b^2} \|f\|_{H_k^2}^2.$$

With this Eq. (A.8) gives

$$\frac{1}{2} \frac{d}{dt} \left\| \partial^2 f \right\|_{L^2}^2 \leq C \left(1 + \|U_0\|_{C_b^{2k+2}} + |\mathbf{v}| \right) \|f\|_{H_k^2}^2 + C \|f\|_{H_k^2} \|g\|_{H_k^2},$$

which implies (3.9). $\square$

References

- [1] J. Bartsch, A. Borzì, F. Fanelli, S. Roy, *A theoretical investigation of Brockett's ensemble optimal control problems* Calc. Var 58, 162 (2019).
- [2] M. A. Alonso, *Wigner functions in optics: describing beams as ray bundles and pulses as particle ensembles*, Advances in Optics and Photonics, 3 (2011), 272–365.
- [3] A. Arnold, C. Ringhofer, *An operator splitting method for the Wigner-Poisson problem*, SIAM journal on numerical analysis, 33 (1996), 1622–1643.

- [4] L. Barletti, *A mathematical introduction to the Wigner formulation of quantum mechanics*, Bollettino dell'Unione Matematica Italiana, 6 (2003), 693–716.
- [5] J. Bartsch, G. Nastasi, and A. Borzì, *Optimal control of the Keilson-Storer master equation in a Monte Carlo framework*, Journal of Computational and Theoretical Transport, 50 (2021), 454–482.
- [6] J. Bartsch, A. Borzì, F. Fanelli, S. Roy, A numerical investigation of Brockett's ensemble optimal control problems, Numerische Mathematik, 149 (2021), 1–42.
- [7] V. Bonačić-Koutecký and R. Mitrić, Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters: Analysis and Control, Chemical Reviews, 105 (2005), 11–66.
- [8] A. Borzì, G. Ciaramella and M. Sprengel, Formulation and Numerical Solution of Quantum Control Problems, SIAM, Philadelphia, 2017.
- [9] A. Borzì, V. Schulz, *Computational Optimization of Systems Governed by Partial Differential Equations.*, vol. 8 of Computational science and engineering, SIAM, 2012.
- [10] R.W. Brockett, *Notes on the control of the Liouville equation*, in Control of partial differential equations, vol. 2048 of Lecture Notes in Math., Springer, Heidelberg, 2012, 101–129.
- [11] V.D. Camiola, G. Mascali, and V. Romano, Charge Transport in Low Dimensional Semiconductor Structures: The Maximum Entropy Approach, Springer International Publishing, 2020
- [12] W. B. Case, *Wigner functions and Weyl transforms for pedestrians*, American Journal of Physics, 76 (2008), 937–946.
- [13] L. Chai, S. Jin, Q. Li, O. Morandi, *A multiband semiclassical model for surface hopping quantum dynamics.*, Multiscale Modeling & Simulation, 13 (2015), 205–230.
- [14] L. Barletti, The two-spin model of a tracking chamber: a phase-space perspective. Journal of Computational Electronics, 20, 2159–2169 (2021)
- [15] Luigi Barletti, Paolo Bordone, Lucio Demeio, Elisa Giovannini Wigner function with correlation damping. Physical Review E, 104, 044112 (2021).
- [16] L. Barletti, G. Frosali, E. Giovannini, Adding decoherence to the Wigner equation. Journal of Computational and Theoretical Transport, 47, 209–225 (2018).
- [17] A. Dorda, F. Schürer, *A WENO-solver combined with adaptive momentum discretization for the Wigner transport equation and its application to resonant tunneling diodes*, Journal of Computational Physics, 284 (2015), 95–116.
- [18] D. Dragoman, *Applications of the Wigner distribution function in signal processing.*, EURASIP J. Adv. Sig. Proc., 2005 (2005), 1520–1534.
- [19] E. J. Heller, *Wigner phase space method: Analysis for semiclassical applications*, The Journal of Chemical Physics, 65 (1976), 1289–1298.
- [20] U. Hohenester, P.K. Rekdal, A. Borzì, J. Schmiedmayer, Optimal quantum control of Bose-Einstein condensates in magnetic microtraps, Phys. Rev. A 75, 023602 (2007).
- [21] C. Jacoboni, A. Bertoni, P. Bordone, R. Brunetti, *Wigner-function formulation for quantum transport in semiconductors: theory and Monte Carlo approach*, Mathematics and computers in simulation, 55 (2001), 67–78.

- [22] A. Jüngel, *Transport Equations for Semiconductors*, Lecture Notes in Physics No. 773, Springer, Berlin, 2009.
- [23] J. Körner, A. Borzi, *Second-order analysis of Fokker–Planck ensemble optimal control problems*, ESAIM: COCV, 28 (2022), 77.
- [24] A. Lubk, F. Röder, *Semiclassical tem image formation in phase space*, Ultramicroscopy, 151 (2015), 136–149.
- [25] G. Manfredi, O. Morandi, L. Friedland, T. Jenke, H. Abele, Chirped-frequency excitation of gravitationally bound ultracold neutrons, Phys. Rev. D 95, 025016 (2017).
- [26] P. A. Markowich, H. Neunzert, *On the equivalence of the Schrödinger and the quantum Liouville equations*, Mathematical Methods in the Applied Sciences, 11 (1989), 459–469.
- [27] F. McLafferty, On quantum trajectories and an approximation to the Wigner path integral, The Journal of Chemical Physics, 83 (1985), 5043–5045.
- [28] O. Morandi, On the connection between the Wigner and the Bohm quantum formalism, Physics Letters A 443, 128223 (2022).
- [29] O. Morandi, Effective classical Liouville-like evolution equation for the quantum phase-space dynamics, J. Phys. A: Math. Theor. 43, 365302 (2010).
- [30] O. Morandi, Quantum corrected Liouville model: mathematical analysis, J. Math. Phys. 53, 063302 (2012).
- [31] O. Morandi and F. Schuerrer, Wigner model for quantum transport in graphene, J. Phys. A: Math. Theor. 44, 265301 (2011).
- [32] A. Mukherjee, A. Bose, M. S. Janaki, *Quantum corrections to nonlinear ion acoustic wave with landau damping*, Physics of Plasmas (1994-present), 21 (2014), 072303.
- [33] T. Paul, P.-L. Lions, *Sur les mesures de Wigner.*, Revista matemática iberoamericana, 9 (1993), 553–618.
- [34] C. Ringhofer, *A spectral method for the numerical simulation of quantum tunneling phenomena*, SIAM Journal on Numerical Analysis, 27 (1990), 32–50.
- [35] S. Roy, A. Borzi, A. Habbal, Pedestrian motion modelled by Fokker - Planck Nash games, Royal Society open science, 4: 170648, 2017.
- [36] S. Shao, T. Lu, W. Cai, *Adaptive conservative cell average spectral element methods for transient Wigner equation in quantum transport*, Commun. Comput. Phys, 9 (2011), 711–739.
- [37] V. I. Tatarskii, *The Wigner representation of quantum mechanics*, Physics-Uspekhi, 26 (1983), 311–327.
- [38] J. Weinbub, M. Ballicchia, M. Nadjalkov, *Gate-controlled electron quantum interference logic*, Nanoscale, 14 (2022), 13520.
- [39] H. Weyl, *Quantenmechanik und Gruppentheorie*, Zeitschrift für Physik, 46 (1927), 1–46.
- [40] E. Wigner, *On the quantum correction for thermodynamic equilibrium*, Physical Review, 40 (1932), 749–759.
- [41] H.M. Wiseman, Quantum trajectories and quantum measurement theory, Quantum and Semiclassical Optics: Journal of the European Optical Society Part B, 8 (1996), 205–222.

- [42] C.K. Zachos, D.B. Fairlie, T.L. Curtright, (eds.) *Quantum mechanics in phase space. An overview with selected papers.* World Scientific Publishing, Hackensack NJ (2005)
- [43] C. Zagoya, J. Wu, M. Ronto, D. V. Shalashilin, C. F. de Morisson Faria, *Quantum and semiclassical phase-space dynamics of a wave packet in strong fields using initial-value representations*, New Journal of Physics, 16 (2014), 103040.
- [44] W. H. Zurek, *Decoherence and the Transition from Quantum to Classical—Revisited*, Los Alamos Science, 27 (2002), 2–25.