

Minimal time for the bilinear control of Schrödinger equations

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Abstract

We consider a quantum particle in a potential $V(x)$ ($x \in \mathbb{R}^N$) subject to a (spatially homogeneous) time-dependent electric field $E(t)$, which plays the role of the control. Under generic assumptions on V , this system is approximately controllable on the $L^2(\mathbb{R}^N, \mathbb{C})$ -sphere, in sufficiently large times T , as proved by Boscain, Caponigro, Chambrion and Sigalotti [1]. In the present article, we show that this approximate controllability result is false in small time. As a consequence, the result by Boscain et al. is, in some sense, optimal with respect to the control time T .

Keywords: Schrödinger equation, quantum control, minimal time.

1. Introduction

1.1. Main result

In this article, we consider quantum systems whose dynamics can be described by a linear Schrödinger equation of the form

$$\begin{cases} i\partial_t\psi(t, x) = \left(-\frac{1}{2}\Delta + V(x) - \langle E(t), x \rangle \right) \psi(t, x), & (t, x) \in (0, T) \times \mathbb{R}^N, \\ \psi(0, x) = \psi_0(x), & x \in \mathbb{R}^N. \end{cases} \quad (1)$$

Here, $N \in \mathbb{N}^*$ is the space dimension, $\langle \cdot, \cdot \rangle$ is the usual scalar product on \mathbb{R}^N , $V : x \in \mathbb{R}^N \rightarrow \mathbb{R}$, $E : t \in (0, T) \rightarrow \mathbb{R}^N$ and $\psi : (t, x) \in (0, T) \times \mathbb{R}^N \rightarrow \mathbb{C}$ are a static potential, a time-dependent electric field, and the wave function,

respectively. This equation represents a quantum particle in the potential V subject to the electric field $E(t)$. Planck's constant and the particle mass have been set to one.

System (1) is a control system in which the state is the wave function ψ , that belongs to the unitary $L^2(\mathbb{R}^N, \mathbb{C})$ -sphere, denoted by \mathcal{S} ; and the control is the electric field E . Such systems have applications in modern technologies such as nuclear magnetic resonance, quantum chemistry and quantum information science. The expression ‘‘bilinear control’’ refers to the bilinear nature of the term $\langle E(t), x \rangle \psi$ with respect to (E, ψ) .

We are interested in the minimal time required to achieve approximate controllability of system (1). Since in (1) decoherence is neglected, in realistic scenarios the model may only be applicable for small times t (typically on the order of several periods of the ground state). Thus, to be practically relevant, controllability results need to be valid for time intervals for which equation (1) remains a reasonable model. Therefore quantification of the minimal control time is an important issue.

First, we recall a classical well-posedness result [2], which we quote from [3]. We consider potentials V that are smooth and subquadratic, i.e.

$$V \in C^\infty(\mathbb{R}^N) \text{ and, } \forall \alpha \in \mathbb{N}^N \text{ such that } |\alpha| \geq 2, \partial_x^\alpha V \in L^\infty(\mathbb{R}^N). \quad (2)$$

Proposition 1. *Consider V satisfying assumption (2) and $E \in L_{loc}^\infty(\mathbb{R}, \mathbb{R}^N)$. There exists a strongly continuous map $(t, s) \in \mathbb{R}^2 \mapsto U(t, s)$, with values in the set of unitary operators on $L^2(\mathbb{R}^N, \mathbb{C})$, such that*

$$U(t, t) = Id, \quad U(t, \tau)U(\tau, s) = U(t, s), \quad U(t, s)^* = U(s, t)^{-1}, \quad \forall t, \tau, s \in \mathbb{R}$$

and for every $t, s \in \mathbb{R}$, $\varphi \in L^2(\mathbb{R}^N, \mathbb{C})$, the function $\psi(t, x) := U(t, s)\varphi(x)$ is a weak solution in $C^0([0, T], L^2(\mathbb{R}^N, \mathbb{C}))$ of the first equation of (1) with initial condition $\psi(s, x) = \varphi(x)$.

For V satisfying (2), we introduce the operator

$$D(A_V) := \left\{ \varphi \in L^2(\mathbb{R}^N); -\frac{1}{2}\Delta\varphi + V(x)\varphi \in L^2(\mathbb{R}^N) \right\}, \\ A_V\varphi := -\frac{1}{2}\Delta\varphi + V(x)\varphi.$$

For appropriate potentials V , approximate controllability of (1) in \mathcal{S} (possibly in large time) is a corollary of a general result by Boscain, Caponigro, Chambrion, Mason and Sigalotti (the original proof of [4] is generalized in

[1]; inequality (4) below is proved in [4, Proposition 4.6]; an analogous statement for vector valued controls is given in [5, Theorem 2.6]; see also [6] for a survey of results in this area).

Theorem 1. *Let $m \in \{1, \dots, N\}$. We assume that*

- *there exists a Hilbert basis $(\phi_k)_{k \in \mathbb{N}}$ of $L^2(\mathbb{R}^N, \mathbb{C})$ composed of eigenvectors of A_V : $A_V \phi_k = \lambda_k \phi_k$ and $x_m \phi_k \in L^2(\mathbb{R}^N)$, $\forall k \in \mathbb{N}$,*
- *$\int_{\mathbb{R}^N} x_m \phi_j(x) \phi_k(x) dx = 0$ for every $j, k \in \mathbb{N}$ such that $\lambda_j = \lambda_k$ and $j \neq k$,*
- *for every $j, k \in \mathbb{N}$, there exists a finite number of integers $p_1, \dots, p_r \in \mathbb{N}$ such that*

$$p_1 = j, \quad p_r = k, \quad \int_{\mathbb{R}^N} x_m \phi_{p_l}(x) \phi_{p_{l+1}}(x) dx \neq 0, \forall l = 1, \dots, r-1, \\ |\lambda_L - \lambda_M| \neq |\lambda_{p_l} - \lambda_{p_{l+1}}|, \forall 1 \leq l \leq r-1, L, M \in \mathbb{N} \text{ with } \{L, M\} \neq \{p_l, p_{l+1}\}.$$

Then, for every $\epsilon > 0$ and $\psi_0, \psi_f \in \mathcal{S}$, there exist a time $T > 0$ and a piecewise constant function $u : [0, T] \rightarrow \mathbb{R}$ such that the solution of (1) with $E(t) = u(t)e_m$ satisfies

$$\|\psi(T) - \psi_f\|_{L^2(\mathbb{R}^N)} < \epsilon. \quad (3)$$

Moreover, for every $\delta > 0$, the existence of a piecewise constant function $u : [0, T] \rightarrow (-\delta, \delta)$ such that the solution of (1) with $E(t) = u(t)e_m$ satisfies (3) implies that

$$T \geq \frac{1}{\delta} \sup_{k \in \mathbb{N}} \frac{||\langle \phi_k, \psi_0 \rangle| - |\langle \phi_k, \psi_f \rangle|| - \epsilon}{\|x_m \phi_k\|_{L^2(\mathbb{R}^N)}}. \quad (4)$$

To prove this statement, the authors use finite dimensional techniques applied to the Galerkin approximations of equation (1). They also prove an estimate on the L^1 -norm of the control [1, Proposition 2.8] and approximate controllability in the sense of density matrices [1, Theorem 2.11].

In Theorem 1, the time T is not known a priori and may be large. Note that the lower bound on the control time in (4) goes to zero when $\delta \rightarrow +\infty$. Thus, approximate controllability *in arbitrarily small time* (allowing potentially large controls) is an open problem. The goal of this article is to prove that, for potentials V satisfying (2), approximate controllability does not hold in arbitrarily small time, even with large controls, as stated in the following theorem.

Theorem 2. Consider V satisfying assumption (2). Let $b > 0$, $x_0, \dot{x}_0 \in \mathbb{R}^N$ and $\psi_0 \in \mathcal{S}$ be defined by

$$\psi_0(x) := \frac{b^{N/4}}{C_N} e^{-\frac{b}{2}\|x-x_0\|^2 + i\langle \dot{x}_0, x-x_0 \rangle} \quad (5)$$

where

$$C_N := \left(\int_{\mathbb{R}^N} e^{-\|y\|^2} dy \right)^{1/2}.$$

Let $\psi_f \in \mathcal{S}$ a state that does not have a Gaussian profile in the sense that

$$|\psi_f(\cdot)| \neq \frac{\det(S)^{1/4}}{C_N} e^{-\frac{1}{2}\|\sqrt{S}(\cdot-\gamma)\|^2}, \quad \forall \gamma \in \mathbb{R}^N, S \in \mathcal{M}_N(\mathbb{R}) \text{ symmetric positive.}$$

Then there exist $T^{**} = T^{**}(\|V''\|_\infty, \|V^{(3)}\|_\infty, b, \psi_f) > 0$ and $\delta = \delta(\|V''\|_\infty, b, \psi_f) > 0$ such that, for every $E \in C_{pw}^0([0, T^{**}], \mathbb{R}^N)$ (piecewise continuous functions $[0, T^{**}] \rightarrow \mathbb{R}^N$), the solution ψ of (1) satisfies

$$\|\psi(t) - \psi_f\|_{L^2(\mathbb{R}^N)} > \delta, \quad \forall t \in [0, T^{**}].$$

In particular, if V satisfies (2) and the assumptions of Theorem 1 (which hold generically, this fact may be proved as in [7]), then system (1) is approximately controllable in \mathcal{S} in large time but not in small time $T < T^{**}$. In this sense, Theorem 1 is optimal with respect to the time of control. A characterization of the minimal time required for ϵ -approximate controllability is an open problem.

1.2. Bibliographical comments

1.2.1. Small-time control and minimal time for ODEs and PDEs

We introduce the finite dimensional bilinear system

$$\frac{dX}{dt}(t) = AX(t) + \sum_{j=1}^m u_j(t) B_j X(t) \quad (6)$$

where $N, m \in \mathbb{N}^*$, $t \mapsto X(t)$ takes values in the unit sphere \mathbb{S}^{2N-1} of \mathbb{C}^N , $A, B_1, \dots, B_m \in su(N) := \{M \in \mathcal{M}_N(\mathbb{C}); \overline{M}^T + M = 0 \text{ and } \text{tr}(M) = 0\}$, with B_1, \dots, B_m linearly independent, and u_1, \dots, u_m are real valued scalar controls. We denote by \mathcal{U} the set of piecewise continuous vector valued controls $u = (u_j)_{1 \leq j \leq m}$. Note that the Galerkin approximations of the Schrödinger

PDE (1) fit in this framework, when the control of the global phase is not required (trace condition). For every $u \in \mathcal{U}$, we denote by $t \mapsto R_u(t)X_0$ the unique solution of (6) with initial condition $X_0 \in \mathbb{S}^{2N-1}$ at time $t = 0$.

The controllability of system (6) may be studied at two different levels:

- at the sphere level, i.e. with state $X(t) \in \mathbb{S}^{2N-1}$ and reachable set

$$\mathcal{A}_{X_0}(T) := \{R_u(t)X_0; u \in \mathcal{U}, 0 \leq t \leq T\} \subset \mathbb{S}^{2N-1}, \quad \forall X_0 \in \mathbb{S}^{2N-1}$$

- at the group level, i.e. with state $R_u(t) \in SU(N) := \{M \in \mathcal{M}_N(\mathbb{C}); \overline{M}^T M = I_N \text{ and } \det(M) = 1\}$ and reachable set

$$\mathcal{A}(T) := \{R_u(t); u \in \mathcal{U}, 0 \leq t \leq T\} \subset SU(N).$$

This second controllability notion is stronger than the first one: $\mathcal{A}(T) = SU(N) \Rightarrow \mathcal{A}_{X_0}(T) = \mathbb{S}^{2N-1}, \forall X_0 \in \mathbb{S}^{2N-1}$

At the group level, system (6) is globally exactly controllable in $SU(N)$ if and only if the Lie algebra generated by $\{A, B_1, \dots, B_m\}$ is $su(N)$: $\mathcal{L}(A, B_1, \dots, B_m) = su(N)$. Then, the minimal control time

$$\rho := \inf\{\tau > 0; \overline{\mathcal{A}(\tau)} = SU(N)\}$$

can be zero or positive, depending on the situation. For instance

- if $\mathcal{L}(B_1, \dots, B_m) = su(N)$, then $\rho = 0$;
- if A does not belong to the ideal in $\mathcal{L}(A, B_1, \dots, B_m)$ generated by $\{B_1, \dots, B_m\}$, then $\rho > 0$ (see [8, Proposition 2.1]); note that this is the case when $m = 1$ and $N \geq 2$.

At the vector level, a necessary and sufficient condition (which is weaker than “ $\mathcal{L}(A, B_1, \dots, B_m) = su(N)$ ”) for the global exact controllability of (6) on the sphere \mathbb{S}^{2N-1} is given in [9, Theorem 1]. Moreover, the minimal time for this global controllability on \mathbb{S}^{2N-1} is zero if and only if there exists a point $Y \in \mathbb{S}^{2N-1}$ such that the evaluation of the Lie algebra generated by B_1, \dots, B_m at this point Y is the tangent space to the sphere at point Y : $\mathcal{L}_Y(B_1, \dots, B_m) = T_Y \mathbb{S}^{2N-1}$ (see [10]).

Moreover, for a given $X_0 \in \mathbb{S}^{2N-1}$, the minimal control time (also called “temporal diameter”)

$$\rho_{X_0} := \inf\{\tau > 0; \overline{\mathcal{A}_{X_0}(\tau)} = \mathbb{S}^{2N-1}\}$$

can be positive, for instance when $m = 1$ and $N \geq 2$ ¹ and then ρ_{X_0} is estimated in [11].

Analogue characterizations and estimates of the minimal time for Schrödinger PDE (1) are widely open problems.

In [12], Boussaïd, Caponigro and Chambrion present an example of a bilinear conservative system in infinite dimension for which approximate controllability holds in arbitrary small times. Thus, under the assumptions of Theorem 1, some systems are approximately controllable in arbitrary small time (see [12]), while others are not (see Theorem 2). A characterization of small time approximately controllable PDEs (1) is a challenging open problem.

1.2.2. Minimal time for local exact controllability with small controls

A different notion of ‘minimal time’ is investigated in [13]. This article focuses on exact controllability and small controls to realize small motions, whereas the present article investigates approximate controllability, large controls E and large motions. Generalizing [14], the authors of [13] describe a general scenario for local exact controllability (with small controls) to hold in large time, but not in small time (barrier). This positive minimal time is related to the loss of directions of the linearized system and the behavior of the second order term in the power series expansion of the solution.

¹A simple proof of this statement is the following one. Up to a change of orthonormal basis in \mathbb{C}^N , one may assume that B_1 is diagonal. Then the components of $X(t)$ and $Y(t) := \exp[-B_1 \int_0^t u_1(s) ds]X(t)$ have the same modulus. For $X_0 \in \mathbb{S}^{2N-1}$ and $j \in \{1, \dots, N\}$ such that $\langle X_0, e_j \rangle \neq 0$, we have

$$\begin{aligned} |\langle X(t), e_j \rangle| - |\langle X_0, e_j \rangle| &= |\langle Y(t), e_j \rangle| - |\langle Y(0), e_j \rangle| \\ &\leq \left| \int_0^t \langle \exp[-B_1 \int_0^\tau u_1] AX(\tau), e_j \rangle d\tau \right| \leq \|A\|t, \end{aligned}$$

which precludes global exact controllability on \mathbb{S}^{2N-1} in small time.

1.3. Notation

Denote by $\mathcal{M}_N(\mathbb{K})$ the set of $N \times N$ matrices with coefficients in $\mathbb{K} = \mathbb{R}$ or \mathbb{C} and I_N its identity element; $\text{Tr}(M)$ the trace of a matrix $M \in \mathcal{M}_N(\mathbb{C})$; $\mathcal{S}_N(\mathbb{R})$ (resp. $\mathcal{S}_N^+(\mathbb{R})$) the set of symmetric matrices (resp. positive symmetric matrices) in $\mathcal{M}_N(\mathbb{R})$; $A \leq B$ when $A, B \in \mathcal{S}_N(\mathbb{R})$ and $B - A \in \mathcal{S}_N^+(\mathbb{R})$; $\|\cdot\|$ the Euclidean norm on \mathbb{R}^N and the associated operator norm on $\mathcal{M}_N(\mathbb{R})$; $\dot{x}(t) := \frac{dx}{dt}(t)$, $\ddot{x}(t) := \frac{d^2x}{dt^2}(t)$, for a function x of the variable t ; $C_{pw}^0([0, T], \mathbb{R}^N)$ the piecewise continuous functions $[0, T] \rightarrow \mathbb{R}^N$; \mathcal{S} the unit sphere in $L^2(\mathbb{R}^N, \mathbb{C})$; (e_1, \dots, e_N) the canonical basis of \mathbb{C}^N and $\langle x, y \rangle := \sum_{i=1}^N x_i y_i$, for every $x = (x_1, x_2, \dots, x_n) \in \mathbb{C}^N$, $y = (y_1, y_2, \dots, y_n) \in \mathbb{C}^N$. Note that this scalar product is complex valued and does not involve conjugation, which is important in dealing with symmetric (not hermitian) complex matrices.

2. Proof of Theorem 2

Let V satisfying (2), $b > 0$, $x_0, \dot{x}_0 \in \mathbb{R}^N$ and ψ_0 defined by (5).

Our strategy to prove Theorem 2, outlined in [15], is semi-classical: it relies on Gaussian approximate solutions that are localized around classical trajectories. They are called ‘trajectory-coherent states’ (TCS) and were originally introduced by Bagrov et al. [16, 17, 18, 19] (for recent and comprehensive mathematical treatments, see [20, 21]). They generalize the well-known explicit solutions for the harmonic oscillator potential $V(x) = x^2$ (see e.g. [22, 23, 24]) and may also be viewed as generalized WKB states.

The approximate solutions $\tilde{\psi} = \tilde{\psi}(t, x)$ (defined in eq. (14) below) depend on functions $x_c : \mathbb{R} \rightarrow \mathbb{R}^N$ and $Q : \mathbb{R} \rightarrow \mathcal{M}_N(\mathbb{C})$, which satisfy the ODEs (7) below. The vector function $x_c(t)$ is the classical (controlled) trajectory satisfying Newton’s equation of motion (7), which includes the control field $E(t)$.

The remainder of this section is organized as follows. In Section 2.1, we prove a preliminary result for the solutions $\tilde{Q}(t)$ of (7). In Section 2.2, we introduce the explicit approximate solution $\tilde{\psi}$ and prove that the error $\|\psi - \tilde{\psi}\|_{L^\infty((0, T), L^2(\mathbb{R}^N))}$ can be bounded uniformly with respect to $E \in C_{pw}^0(\mathbb{R}, \mathbb{R}^N)$. Finally, Section 2.3 contains the proof of Theorem 2.

2.1. The ODE for $Q(t)$

For $E \in C_{pw}^0(\mathbb{R}, \mathbb{R}^N)$, we introduce the maximal solutions $x_c \in C^1 \cap C_{pw}^2(\mathbb{R}, \mathbb{R}^N)$ and $Q \in C^1((T^-, T^+), \mathcal{M}_N(\mathbb{C}))$ of

$$\begin{cases} \frac{d^2 x_c}{dt^2}(t) + \nabla V[x_c(t)] = E(t), \\ x_c(0) = x_0, \\ \frac{dx_c}{dt}(0) = \dot{x}_0, \end{cases} \quad \begin{cases} \frac{dQ}{dt}(t) + Q(t)^2 + V''[x_c(t)] = 0, \\ Q(0) = ibI_N, \end{cases} \quad (7)$$

where ∇V and V'' denote the gradient and Hessian matrix of V , respectively. Note that x_c is defined for every $t \in \mathbb{R}$ because ∇V is globally Lipschitz by assumption (2); and the complex coefficient matrix $Q(t)$ is symmetric for every $t \in (T^-, T^+)$, so $Q_2(t) := \Im[Q(t)]$ is symmetric as well. A priori, the maximal interval (T^-, T^+) may depend on E .

Proposition 2. *There exists $T^* = T^*(b, \|V''\|_\infty) > 0$ such that, for every $E \in C_{pw}^0(\mathbb{R}, \mathbb{R}^N)$, $Q(t)$ is defined for every $t \in [0, T^*]$ (i.e. $T^+ > T^*$) and*

$$\frac{b}{2}I_N \leq Q_2(t) \leq \frac{3b}{2}I_N, \text{ for every } t \in [0, T^*]. \quad (8)$$

Proof of Proposition 2: Let $T^* = T^*(b, \|V''\|_\infty) > 0$ be such that

$$t[1 + b^2 e^{4t} + \|V''\|_\infty] < 1 \quad \text{and} \quad 2te^{2t} \leq \frac{1}{2}, \quad \forall t \in [0, T^*]. \quad (9)$$

Step 1: Equations satisfied by $Q_1(t) := \Re[Q(t)]$ and $Q_2(t) := \Im[Q(t)]$. Since V'' is real, (7) implies, on (T^-, T^+)

$$\begin{cases} \frac{dQ_1}{dt} + Q_1^2 - Q_2^2 + V''[x_c] = 0, \\ Q_1(0) = 0, \end{cases} \quad \begin{cases} \frac{dQ_2}{dt} + Q_1Q_2 + Q_2Q_1 = 0, \\ Q_2(0) = bI_N. \end{cases} \quad (10)$$

By Gronwall lemma and (10),

$$\|Q_2(t)\| \leq be^{2 \int_0^t \|Q_1(s)\| ds}, \quad \forall t \in [0, T^+]. \quad (11)$$

Step 2: We prove that $T^+ > T^*$ for every $E \in C_{pw}^0(\mathbb{R}, \mathbb{R}^N)$. Working by contradiction, we assume the existence of $E \in C_{pw}^0(\mathbb{R}, \mathbb{R}^N)$ such that $T^+ < T^*$. In particular T^+ is finite, thus $Q(t)$ explodes as $t \rightarrow T^+$. We then deduce from (11) that $Q_1(t)$ explodes as $t \rightarrow T^+$. Thus

$$t^* := \sup\{t \in [0, T^+); \|Q_1(s)\| \leq 1, \forall s \in [0, t]\} \quad (12)$$

belongs to $(0, T^+)$ and $\|Q_1(t^*)\| = 1$. Now we have

$$\begin{aligned} 1 &= \|Q_1(t^*)\| = \left\| \int_0^{t^*} \left(-Q_1(s)^2 + Q_2(s)^2 - V''[x_c(s)] \right) ds \right\| \quad \text{by (10)} \\ &\leq \int_0^{t^*} \left(\|Q_1(s)\|^2 + b^2 e^{4 \int_0^s \|Q_1(s)\| ds} + \|V''[x_c(s)]\| \right) ds \quad \text{by (11)} \\ &\leq t^* [1 + b^2 e^{4t^*} + \|V''\|_\infty] < 1 \quad \text{by (12) and (9),} \end{aligned}$$

which is a contradiction. Therefore $T^+ > T^*$ for every $E \in C_{pw}^0(\mathbb{R}, \mathbb{R}^N)$.

Step 3: Conclusion. The same argument proves that $t^* > T^*$, i.e. $\|Q_1(t)\| \leq 1$ for every $t \in [0, T^*]$. Thus, by (10), (11) and (9) we have

$$\|Q_2(t) - bI_N\| = \left\| \int_0^t [Q_2 Q_1 + Q_1 Q_2](s) ds \right\| \leq 2t b e^{2t} < \frac{b}{2}, \forall t \in [0, T^*].$$

2.2. Approximate solution

We introduce the ‘classical action’ $S : (t, x) \in \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}$

$$S(t, x) := \int_0^t \left(\frac{1}{2} \|\dot{x}_c(s)\|^2 - V[x_c(s)] \right) ds + \langle \dot{x}_c(t), x - x_c(t) \rangle \quad (13)$$

and the approximate solution

$$\begin{aligned} \tilde{\psi}(t, x) &:= \frac{b^{N/4}}{C_N} \exp \left[\Phi(t, x) \right] \quad \text{where} \\ \Phi(t, x) &:= i \left(S(t, x) + \frac{1}{2} \langle Q(t)[x - x_c(t)], x - x_c(t) \rangle \right) + \\ &\quad \int_0^t \left(i \langle x_c(s), E(s) \rangle - \frac{\text{Tr}[Q(s)]}{2} \right) ds. \end{aligned} \quad (14)$$

Note that equation (10) ensures that $\tilde{\psi}(t) \in \mathcal{S}$. Indeed, for every $t \in (0, T^*)$,

$$\begin{aligned} \frac{d}{dt} \det[Q_2(t)] &= \det[Q_2(t)] \text{Tr} \left[Q_2(t)^{-1} \dot{Q}_2(t) \right] \\ &= \det[Q_2(t)] \text{Tr} \left[Q_2(t)^{-1} \left(-Q_1(t) Q_2(t) - Q_2(t) Q_1(t) \right) \right] \\ &= -2 \text{Tr}[Q_1(t)] \det[Q_2(t)], \end{aligned}$$

which, together with (10), implies that

$$\det[Q_2(t)] = b^N e^{-2 \int_0^t \text{Tr}[Q_1(s)] ds}. \quad (15)$$

Therefore,

$$\begin{aligned} \|\tilde{\psi}(t)\|_{L^2(\mathbb{R}^N)} &= \frac{b^{N/4}}{C_N} e^{-\frac{1}{2} \int_0^t \text{Tr}[Q_1(s)] ds} \left(\int_{\mathbb{R}^N} e^{-\langle Q_2(t)[x - x_c(t)], x - x_c(t) \rangle} dx \right)^{1/2} \\ &= \frac{b^{N/4}}{C_N} e^{-\frac{1}{2} \int_0^t \text{Tr}[Q_1(s)] ds} \frac{C_N}{\det[Q_2(t)]^{1/4}} = 1. \end{aligned}$$

Note that, by (15), $Q_2(t)$ is positive for every $t \in (T^-, T^+)$, which legitimizes the previous computations.

Proposition 3. *There exists a constant $C_* > 0$ such that, for every V satisfying (2), $b > 0$, $x_0, \dot{x}_0 \in \mathbb{R}^N$ and $E \in C_{pw}^0(\mathbb{R}, \mathbb{R}^N)$, the solution ψ of (1) with ψ_0 defined by (5) and the function $\tilde{\psi}$ defined by (14) satisfy*

$$\|(\psi - \tilde{\psi})(t)\|_{L^2(\mathbb{R}^N)} \leq C_* \|V^{(3)}\|_\infty \int_0^t \|Q_2(s)^{-1}\|^{3/2} ds, \quad \forall t \in [0, T^*],$$

where T^* is defined in Proposition 2.

Proof of Proposition 3:

Step 1: Equation satisfied by $\tilde{\psi}$. On the one hand, we have (note that S is affine in the variable x)

$$\begin{aligned} \nabla \tilde{\psi} &= i \left(\nabla S + Q[x - x_c] \right) \tilde{\psi}, \\ \Delta \tilde{\psi} &= [-\langle \nabla S + Q[x - x_c], \nabla S + Q[x - x_c] \rangle + i \text{Tr}(Q)] \tilde{\psi} \\ &= [-\langle \dot{x}_c + Q[x - x_c], \dot{x}_c + Q[x - x_c] \rangle + i \text{Tr}(Q)] \tilde{\psi}. \end{aligned}$$

Thus

$$\frac{1}{2} \Delta \tilde{\psi} = \left[-\frac{1}{2} \|\dot{x}_c\|^2 - \langle \dot{x}_c, Q[x - x_c] \rangle - \frac{1}{2} \langle Q^2[x - x_c], [x - x_c] \rangle + \frac{i}{2} \text{Tr}(Q) \right] \tilde{\psi}. \quad (16)$$

On the other hand, we have

$$\begin{aligned} i \partial_t \tilde{\psi} &= \left[-\left(\partial_t S + \frac{1}{2} \langle \dot{Q}[x - x_c], x - x_c \rangle - \langle Q \dot{x}_c, x - x_c \rangle \right) - \frac{i}{2} \text{Tr}(Q) - \langle x_c, E \rangle \right] \tilde{\psi} \\ &= \left[-\frac{1}{2} \|\dot{x}_c\|^2 + V[x_c] - \langle \ddot{x}_c, x - x_c \rangle + \|\dot{x}_c\|^2 - \frac{1}{2} \langle \dot{Q}[x - x_c], x - x_c \rangle \right. \\ &\quad \left. + \langle Q \dot{x}_c, x - x_c \rangle - \frac{i}{2} \text{Tr}(Q) - \langle x_c, E \rangle \right] \tilde{\psi} \\ &= \left[\frac{1}{2} \|\dot{x}_c\|^2 + V[x_c] + \langle \nabla V(x_c) - E, x - x_c \rangle \right. \\ &\quad \left. + \frac{1}{2} \langle [Q^2 + V''(x_c)][x - x_c], x - x_c \rangle + \langle Q \dot{x}_c, x - x_c \rangle \right. \\ &\quad \left. - \frac{i}{2} \text{Tr}(Q) - \langle x_c, E \rangle \right] \tilde{\psi}. \end{aligned} \quad (17)$$

Combining (16) and (17) gives

$$i \partial_t \tilde{\psi}(t, x) + \frac{1}{2} \Delta \tilde{\psi}(t, x) - V(x) \tilde{\psi}(t, x) + \langle E(t), x \rangle \tilde{\psi}(t, x) = r(t, x) \quad (18)$$

where

$$r(t, x) := -\left(V(x) - V(x_c) - \langle \nabla V(x_c), x - x_c \rangle - \frac{1}{2} \langle V''(x_c)[x - x_c], x - x_c \rangle\right) \tilde{\psi}(t, x). \quad (19)$$

Step 2: Conclusion. Using (19), (14) and (15) and Taylor's formula, we get

$$\begin{aligned} \|r(t)\|_{L^2(\mathbb{R}^N)}^2 &\leq \int_{\mathbb{R}^N} \left| \frac{\|V^{(3)}\|_\infty}{3!} \|x - x_c\|^3 \right|^2 \frac{b^{N/2}}{C_N^2} e^{-\langle Q_2(t)[x - x_c], x - x_c \rangle - \int_0^t \text{Tr}(Q_1)} dx \\ &\leq \frac{\|V^{(3)}\|_\infty^2}{(3!)^2 C_N^2} \int_{\mathbb{R}^N} \|x - x_c\|^6 e^{-\langle Q_2(t)[x - x_c], x - x_c \rangle} \sqrt{\det[Q_2(t)]} dx \\ &\leq C_*^2 \|V^{(3)}\|_\infty^2 \|Q_2(t)\|^{-1/2} \|\cdot\|^6, \end{aligned}$$

where

$$C_* := \frac{1}{3! C_N} \left(\int_{\mathbb{R}^N} \|y\|^6 e^{-\|y\|^2} dy \right)^{1/2}.$$

Let $U(t, s)$ be the evolution operator for equation (1) (see Proposition 1). Then,

$$(\psi - \tilde{\psi})(t) = \int_0^t U(t, s) r(s) ds \text{ in } L^2(\mathbb{R}^N), \forall t \in (0, T^*),$$

and $U(t, s)$ is an isometry of $L^2(\mathbb{R}^N)$ for every $t \geq s \geq 0$, thus

$$\|(\psi - \tilde{\psi})(t)\|_{L^2(\mathbb{R}^N)} \leq \int_0^t \|r(s)\|_{L^2(\mathbb{R}^N)} ds \leq \int_0^t C_* \|V^{(3)}\|_\infty \|Q_2(s)\|^{-1} \|\cdot\|^{3/2} ds. \quad (20)$$

□

Remark 1. *The trajectory-coherent states $\tilde{\psi}$ are only approximate solutions to the Schrödinger equation; however, they are exact solutions for quadratic potentials V (see (18) and (19)), which is the key point of reference [24].*

2.3. Proof of the main result

Let $T^* = T^*(b, \|V''\|_\infty) > 0$ be as in Proposition 2. The key point of the proof is the fact that, for every $E \in C_{pw}^0(\mathbb{R}, \mathbb{R})$, the approximate solution $\tilde{\psi}$ has a Gaussian profile. Indeed, from (13), (14) and (15), one has

$$|\tilde{\psi}(t, x)|^2 = \frac{\det[\sqrt{Q_2(t)}]}{C_N^2} e^{-\|\sqrt{Q_2(t)}[x - x_c(t)]\|^2},$$

where $Q_2(t)$ is a real symmetric matrix satisfying (8).

Step 1: We prove that the set

$$\mathcal{V} := \left\{ \phi \in \mathcal{S}; \exists q \in \mathcal{S}_N^+(\mathbb{R}) \text{ with } \sqrt{\frac{b}{2}}I_N \leq q \leq \sqrt{\frac{3b}{2}}I_N \text{ and } \alpha \in \mathbb{R}^N \text{ such that } |\phi(x)|^2 = \frac{\det(q)}{C_N^2} e^{-\|q(x-\alpha)\|^2} \text{ a.e.} \right\}$$

is a strict closed subset of \mathcal{S} .

Clearly, \mathcal{V} is a strict subset of \mathcal{S} . Let $(\phi_n)_{n \in \mathbb{N}}$ be a sequence of \mathcal{V} that converges in $L^2(\mathbb{R}^N, \mathbb{C})$ to $\phi_\infty \in \mathcal{S}$. For every $n \in \mathbb{N}$, we denote by $\alpha_n \in \mathbb{R}^N$ and $q_n \in \mathcal{S}_N^+(\mathbb{R})$ the corresponding parameters; q_n satisfies

$$\sqrt{\frac{b}{2}}I_N \leq q_n \leq \sqrt{\frac{3b}{2}}I_N. \quad (21)$$

By extracting a subsequence if necessary, we may assume w.l.o.g. that $\phi_n(x) \rightarrow \phi_\infty(x)$ for almost every $x \in \mathbb{R}^N$ (Lebesgue).

Step 1.1: Up to a possible extraction of a subsequence, we may assume that $q_n \rightarrow q_\infty$ where $q_\infty \in \mathcal{S}_N^+(\mathbb{R})$ and $\sqrt{\frac{b}{2}}I_N \leq q_\infty \leq \sqrt{\frac{3b}{2}}I_N$. This may be seen by diagonalizing and appealing to the compactness of $O_N(\mathbb{R}) \times [\sqrt{b/2}, \sqrt{3b/2}]^N$.

Step 1.2: Up to a possible extraction of a subsequence, we may assume that $\alpha_n \rightarrow \alpha_\infty \in \mathbb{R}^N$. Working by contradiction, we assume that $(\alpha_n)_{n \in \mathbb{N}}$ is not bounded. We may assume w.l.o.g. that $\|\alpha_n\| \rightarrow +\infty$ when $n \rightarrow \infty$. Then, by (21),

$$|\phi_n(x)|^2 = \frac{\det(q_n)}{C_N^2} e^{-\|q_n(x-\alpha_n)\|^2} \leq \frac{(3b/2)^{N/2}}{C_N^2} e^{-\frac{b}{2}\|x-\alpha_n\|^2} \rightarrow 0 \quad \text{a.e. } x \in \mathbb{R}^N.$$

Thus $\phi_\infty = 0$ (uniqueness of the a.e. limit), which is impossible because $\phi_\infty \in \mathcal{S}$.

Step 1.3: Conclusion. The uniqueness of the a.e. limit gives

$$|\phi_\infty(x)|^2 = \frac{\det(q_\infty)}{C_N^2} e^{-\|q_\infty(x-\alpha_\infty)\|^2} \quad \text{a.e. } x \in \mathbb{R}^N$$

thus $\phi_\infty \in \mathcal{V}$. This concludes Step 1.

Step 2: Let $\psi_f \in \mathcal{S} \setminus \mathcal{V}$ (which holds, in particular, when ψ_f does not have a Gaussian profile). Then $\delta_0 := \text{distance}_{L^2(\mathbb{R}^N, \mathbb{C})}(\psi_f; \mathcal{V}) > 0$. Let

$$T^{**} = T^{**}(\psi_f, b, V) := \min \left\{ T^*; \frac{\delta_0 (b/2)^{3/2}}{2C_* \|V^{(3)}\|_\infty} \right\}.$$

Then, using (8) and (20), we get that, for every $t \in [0, T^{**}]$ and $E \in C_{pw}^0(\mathbb{R}, \mathbb{R})$, the solution ψ of (1) satisfies

$$\begin{aligned} \|\psi_f - \psi(t)\|_{L^2(\mathbb{R})} &\geq \left| \|\psi_f - \tilde{\psi}(t)\|_{L^2(\mathbb{R})} - \|(\tilde{\psi} - \psi)(t)\|_{L^2(\mathbb{R})} \right| \\ &\geq \delta_0 - C_* \|V^{(3)}\|_\infty \frac{t}{(b/2)^{3/2}} \geq \frac{\delta_0}{2}. \quad \square \end{aligned}$$

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