Stability of wave packet dynamics under perturbations

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Abstract

We introduce a novel method to investigate the stability of wave packet dynamics under perturbations of the Hamiltonian. Our approach relies on semiclassical approximations, but is non-perturbative. Two separate contributions to the quantum fidelity are identified: one factor derives from the dispersion of the wave packets, whereas the other factor is determined by the separation of a trajectory of the perturbed classical system away from a corresponding unperturbed trajectory. We furthermore estimate both contributions in terms of classical Lyapunov exponents and find a decay of fidelity that is, generically, at least exponential, but may also be doubly exponential. The latter case is shown to be realised for inverted harmonic oscillators.
1 Introduction

It has long been appreciated that, in contrast to chaotic classical dynamics, the time evolution of a quantum system shows no sensible dependence on initial conditions. This follows immediately from the unitarity of quantum dynamics. Hence, rather than being concerned with instabilities at large times, the notion of quantum chaos is commonly reserved for semiclassical studies that aim at relating statistical properties of stationary quantum states to dynamical properties of chaotic classical systems (see, e.g., [1, 2]). More recently, however, the behaviour of quantum time evolutions at large times has attracted an increasing attention (see, e.g., [3, 4, 5, 6]). Both in the dynamics of observables (Heisenberg picture) and in the evolution of wave functions (Schrödinger picture) it has been proven that there exists a time scale (the so-called Ehrenfest time), depending on the semiclassical parameter $\hbar$, below which the quantum dynamics can be well approximated in terms of the associated classical time evolution. Moreover, if the classical dynamics are chaotic, this time scale is inversely proportional to a suitable classical Lyapunov exponent.

Some time ago Peres suggested [7] that instead of studying the behaviour of quantum dynamics under a change of initial conditions one should investigate its stability under perturbations of the Hamiltonian: Suppose that an initial state $\psi$ is evolved under the unitary dynamics $\hat{U}_0(t)$ generated by the quantum Hamiltonian $\hat{H}_0$, one compares this with the evolution $\hat{U}_\varepsilon(t)\psi$ determined by the perturbed Hamiltonian $\hat{H}_\varepsilon = \hat{H}_0 + \varepsilon\hat{V}$. Here $\hat{V}$ is a perturbation of unit strength, and $\varepsilon$ is a variable parameter. Then the quantum fidelity

$$F(t) = |\langle \psi, \hat{U}_\varepsilon(t)^{-1}\hat{U}_0(t)\psi \rangle|^2$$

measures how sensibly the dynamics reacts to this perturbation. It can also be viewed as a means to quantify to what extent the initial state can be recovered after it has been propagated for a time $t$ with the unperturbed dynamics, and then the time evolution is reversed with a perturbation being turned on. For that reason the quantity (1.1) is also known as quantum Loschmidt echo.

Peres analysed $F(t)$ in perturbation theory, and found an initial decay $F(t) \sim 1 - C_{\hat{V},\psi}(\varepsilon t/\hbar)^2$. Since the reliability of perturbative results requires $\varepsilon t/\hbar$ to be small, one could view Peres’ result as indicating a Gaussian decay of the fidelity on an initial time scale that depends on $\varepsilon$ and $\hbar$. Later work focused on time scales beyond this perturbative regime or on strong perturbations, respectively, and found an exponential decay [8, 9, 10, 11]. Its rate is either determined by Fermi’s golden rule [8] or, for stronger perturbations, by a classical Lyapunov exponent [9, 11]. Further studies related the behaviour of the fidelity to the decay of (quantum as well as classical) correlations [12]. All of these results rest on a number of approximations and assumptions. Hence the precise time scales for the different regimes depend on various factors as, e.g., initial states, strength of perturbation, averages over random perturbations, and dynamical properties of the corresponding classical dynamics.

Here our principal aim is to develop an alternative approach to the decay of quantum fidelity for particular initial states. The method that we shall introduce below is non-perturbative (quantum mechanically as well as classically) and employs only semiclassical
approximations with a rigorous control over the errors. Previous semiclassical studies of fidelity decay used the Van Vleck-Gutzwiller propagator for the time evolution of Gaussian initial states. This procedure takes care of the leading term in an expansion in powers of $\hbar$, with an error that is, formally, smaller by a factor of $\hbar$. For finite times this is indeed true, but there is no analytical control over the semiclassical error that arises in estimates of the fidelity decay at large times. Our method, however, allows to bound the semiclassical error in terms of the linear stability of an associated classical dynamics. It can in particular be applied to Gaussian states. And although our approach requires no particular assumptions about the nature of the classical dynamics, we are mostly interested in the case of chaotic (i.e., exponentially unstable) classical trajectories. In that case we find a decay of fidelity prior to the Ehrenfest time that generically is at least exponential. But it may also be doubly exponential, which we show to be the case in the example of inverted harmonic oscillators.

This paper is organised as follows: In Section 2 we introduce the wave packets that we shall consider as initial states and review their semiclassical dynamics. The decay of quantum fidelity is investigated in Section 3 with an emphasis on the behaviour of Gaussian states. An exact calculation of the fidelity for inverted harmonic oscillators is performed in Section 4. We finally summarise our findings in Section 5. Three appendices are devoted to a number of technical considerations: We first review the metaplectic representation, then discuss a transformation of positive-definite, symmetric matrices to a diagonal form, and finally collect estimates of matrix norms and singular values.

2 Localised wave packets

The initial states to which our approach applies are wave packets with a localisation both in position and momentum. By this we understand a concentration of the quantum state in a suitable phase space representation on a single point, when the semiclassical limit is performed by passing to a small (effective) Planck’s constant $\hbar$. We specify the wave packets in terms of normalised, smooth, and rapidly decreasing functions $\phi(x)$ (Schwartz test functions) of $x \in \mathbb{R}^d$. Examples for this are provided by the Gaussian functions

$$\phi^Z(x) = \left(\frac{\det \text{Im } Z}{\pi^d}\right)^{1/4} e^{\frac{i}{\hbar}xz},$$

where $Z$ is a complex, symmetric $d \times d$ matrix with positive-definite imaginary part.

For the purpose of semiclassical investigations we introduce the scaling

$$\phi^h(x) = h^{-d/4}\phi\left(x/\sqrt{\hbar}\right).$$

This produces quantum states that are semiclassically concentrated at zero in position and in momentum. Such a phase space localisation is best analysed in the Wigner representation

$$W[\phi^h](\xi, x) = \int \phi^h(x - \frac{y}{2}) \phi^h(x + \frac{y}{2}) e^{-\frac{i}{\hbar}y \cdot \xi} dy.$$
which, if multiplied by \((2\pi\hbar)^{-d}\), converges to \(\delta(\xi, x)\) as \(\hbar \to 0\). A subsequent application of the phase space translation

\[
\hat{D}(p, q) = e^{-\frac{i}{\hbar}q \cdot \hat{P} - p \cdot \hat{Q}}
\]

(2.4)

therefore yields a wave packet

\[
\phi^h_{(p, q)}(x) = e^{-\frac{i}{\hbar}p \cdot q} \hat{D}(p, q) \phi^h(x) = e^{\frac{i}{\hbar}p \cdot (x - q)} \phi^h(x - q)
\]

(2.5)

with phase space localisation at the point \((p, q)\). The phase convention made here is introduced for convenience; it merely simplifies some of the expressions below.

The time evolution of such a state, generated by a quantum Hamiltonian \(\hat{H}\) that arises as a Weyl quantisation of a classical Hamiltonian \(H(p, q)\),

\[
\hat{H} \psi(x) = \int \int H(p, \frac{x+y}{2}) e^{\frac{i}{\hbar}p \cdot (x-y)} \psi(y) \frac{dp dy}{(2\pi\hbar)^d},
\]

(2.6)

can be determined semiclassically \([14, 3]\) to be

\[
\hat{U}(t) \phi^h_{(p, q)} = e^{\frac{i}{\hbar}R_t \hat{D}(p_t, q_t)} \hat{\mu}(S_t) \phi^h + O_t(\sqrt{\hbar}).
\]

(2.7)

The main term on the r.h.s. is again a wave packet of the type (2.5), but now localised at \((p_t, q_t)\). This is the point on the trajectory emerging in time \(t\) from the initial point \((p, q)\) under the classical dynamics generated by the Hamiltonian \(H(p, q)\). Moreover,

\[
R_t = \int_0^t (\dot{q}_s \cdot \dot{p}_s - H(p_s, q_s)) \, ds
\]

(2.8)

is the action of this trajectory and \(S_t\) is the associated stability matrix. This is a real, symplectic \(2d \times 2d\) matrix that arises as a solution of

\[
\dot{S}_t = J H''(p_t, q_t) \, S_t, \quad S_0 = 1.
\]

(2.9)

Here \(J\) is the symplectic unit \([A.3]\) and \(H''(p, q)\) is the Hessian matrix of the Hamiltonian. Equivalently, the stability matrix is given as

\[
S_t = \left(\begin{array}{cc}
\frac{\partial p}{\partial p} & \frac{\partial p}{\partial q} \\
\frac{\partial p}{\partial q} & \frac{\partial q}{\partial q}
\end{array}\right).
\]

(2.10)

The wave packet at time \(t\) on the r.h.s. of (2.7) arises from the initial state \(\phi^h\) through the application of a unitary operator consisting of two contributions: the first factor is the metaplectic operator \(\hat{\mu}(S_t)\) that provides a double valued representation of the symplectic group (of linear canonical transformations), see Appendix \(A\) and \([15, 16, 17]\) for details. As can be drawn from \([A.8]\), a metaplectic operator does not change the semiclassical
phase space localisation. In (2.7) it is rather responsible for the dispersion of the wave packet. The second factor, $\hat{D}(p_i, q_i)$, then provides a translation of the wave packet along the classical trajectory. Finally, the error term $O(t/\sqrt{\hbar})$ stands for a vector whose norm can be estimated from above by $K(t)\sqrt{\hbar}$. The function $K(t) > 0$ contains the linear stability of the trajectory $(p_i, q_i)$. If the latter is exponentially unstable with maximal Lyapunov exponent $\lambda > 0$, the function $K(t)$ grows like $te^{3\lambda t}$ as $t \to \infty$ [3]. Therefore, as long as $t \ll T_E(\hbar)$, with an Ehrenfest time $T_E(\hbar) = |\log \hbar|/6\lambda$, the error term remains small. In contrast, if the trajectory is stable (in an integrable system or on a KAM-torus) the growth of $K(t)$ is algebraic (like $t^4$) and hence $T_E(\hbar) = C \hbar^{-1/8}$. In any case, this finding enables one to extend the validity of the semiclassical evolution (2.7) to infinite times, when $\hbar \to 0$. We remark that the main term in (2.7) actually is the leading contribution in a systematic semiclassical expansion [3]. If this is carried on to the $N$-th term, the error is $O_t(\hbar^{N/2})$ and can also be controlled up to $T_E(\hbar)$.

3 Fidelity decay

The quantum fidelity of an initial wave packet of the type (2.5) can most conveniently be calculated in the Wigner representation,

$$F(t) = |\langle \hat{U}_0(t)\phi^h_{(p,q)}, \hat{U}_\varepsilon(t)\phi^h_{(p,q)} \rangle|^2 = \int \int W[\hat{U}_0(t)\phi^h_{(p,q)}](\xi, x) W[\hat{U}_\varepsilon(t)\phi^h_{(p,q)}](\xi, x) \frac{d\xi dx}{(2\pi\hbar)^d}. \quad (3.1)$$

We now introduce the semiclassical result (2.7) for the perturbed and for the unperturbed time evolution, respectively, to this expression. The corresponding unperturbed and perturbed classical trajectories shall be denoted as $(p_i^0, q_i^0)$ and $(p_i^\varepsilon, q_i^\varepsilon)$. Exploiting the behaviour

$$W[\hat{D}(p, q)\psi](\xi, x) = W[\psi](\xi - p, x - q) \quad (3.2)$$

of a quantum state $\psi$ in the Wigner representation under phase space translations, one may change variables and define $(\delta p_i, \delta q_i) = (p_i^0 - p_i^\varepsilon, q_i^0 - q_i^\varepsilon)$. For the leading semiclassical contribution one thus obtains

$$F_{sc}(t) = \int \int W[\hat{\mu}(S_i^\varepsilon)\phi^h](\xi - \delta p_i, x - \delta q_i) W[\hat{\mu}(S_i^0)\phi^h](\xi, x) \frac{d\xi dx}{(2\pi\hbar)^d}. \quad (3.3)$$

Since semiclassically the Wigner representations of localised wave packets approach $\delta$-functions, after a division by $(2\pi\hbar)^d$ the result (3.3) can be viewed as a smeared out classical fidelity that measures the separation $(\delta p_i, \delta q_i)$ of the perturbed trajectory from the unperturbed one.

For a more detailed study of the expression (3.3) we now restrict ourselves to Gaussian initial states of the form (2.11) with the scaling (2.2). The action of a metaplectic operator on such states can be calculated explicitly [15, 16, 17],

$$\hat{\mu}(S)\phi^{Z,h} = e^{i\frac{\pi}{2}\sigma} \phi^{S[Z],h}. \quad (3.4)$$
Here $S[Z]$ denotes a map, given by the symplectic matrix $S$, on the space of complex, symmetric matrices with positive-definite imaginary part to itself,

$$S[Z] = (AZ + B)(CZ + D)^{-1} , \quad S = \begin{pmatrix} A & B \\ C & D \end{pmatrix} .$$  \hfill (3.5)

Furthermore, $\sigma$ is a Maslov phase defined through

$$e^{i\pi \sigma} = \left( \frac{\det \text{Im} Z}{\det \text{Im} S[Z]} \right)^{1/4} \left( \det (CZ + D) \right)^{-1/2} .$$  \hfill (3.6)

The Wigner transform of such a Gaussian state is well known to be a Gaussian in phase space,

$$W[\phi^Z,\hbar](\xi, x) = 2^d e^{-\frac{1}{\hbar}(\xi,x) G_Z(\xi, x)} ,$$  \hfill (3.7)

where

$$G_Z = \begin{pmatrix} (\text{Im} Z)^{-1} & -(\text{Im} Z)^{-1} \text{Re} Z \\ -\text{Re} Z (\text{Im} Z)^{-1} & \text{Im} Z + \text{Re} Z (\text{Im} Z)^{-1} \text{Re} Z \end{pmatrix}$$  \hfill (3.8)

is a symmetric, symplectic, and positive-definite $2d \times 2d$ matrix with unit determinant. The behaviour of $(3.8)$ under the transformation $(3.5)$ can be inferred from an application of a metaplectic operator to a Gaussian state in the Wigner representation $(3.7)$. This way, from $(3.4)$ and $(A.8)$ one concludes that

$$G_{S[Z]} = (S^{-1})^T G_Z S^{-1} .$$  \hfill (3.9)

Now, $(3.3)$ is a Gaussian integral that can immediately be evaluated, and the result may be factorised according to

$$F_{\text{scl}}(t) = F_{\text{disp}}(t) F_{\text{class}}(t) .$$  \hfill (3.10)

The first factor

$$F_{\text{disp}}(t) = \left( \det \left( G_{S^0[Z]} + G_{S^\varepsilon[Z]} \right) \right)^{-1/2}$$  \hfill (3.11)

is determined by the dispersion of the wave packets. This interpretation follows from the fact that setting $\delta p_t$ and $\delta q_t$ to zero in $(3.3)$, and therefore removing the phase space translations that arise from $(2.7)$, the integral would exactly yield $(3.11)$. In fact, $F_{\text{disp}}(t)$ measures the differences in the dispersions caused by the two dynamics in question. This contribution is independent of $\hbar$. The time dependence of $(3.11)$ follows from the relation $(3.9)$ with $S^0_t$ and $S^\varepsilon_t$, respectively. It is therefore completely determined by the linear stabilities of the perturbed and the unperturbed classical trajectory. In addition to this, the second factor $F_{\text{class}}(t)$ is influenced by the actual separation $(\delta p_t, \delta q_t)$ of these trajectories. It reads

$$F_{\text{class}}(t) = 2^d \exp \left[ -\frac{1}{\hbar} (\delta p_t, \delta q_t) \cdot G_{S^0[Z]} \left( \mathbb{1} - \Gamma_{t,\varepsilon}^{-1} \right) (\delta p_t, \delta q_t) \right] , \quad \Gamma_{t,\varepsilon} = \mathbb{1} + G_{S^0[Z]}^{-1} G_{S^\varepsilon[Z]}$$  \hfill (3.12)
and, despite of its $\hbar$-dependence, essentially represents a classical fidelity since it is localised on the separation of the classical trajectories: If one divides $F(t)$ by $(2\pi\hbar)^d$ as discussed above, the contributions of (3.11) and (3.12) converge to $\delta(\delta p_i, \delta q_i)$ as $\hbar \to 0$. This also explains the necessity of $\hbar$ in (3.12). We remark that expressions equivalent to (3.10)-(3.12) have independently been obtained by M. Combescure and D. Robert [18].

At this point we stress that in general the separation $(\delta p_i, \delta q_i)$ of the trajectories for large $t$ differs essentially from the corresponding behaviour of the linearised dynamics. In particular, an exponential instability expressed in terms of positive Lyapunov exponents does not imply an exponential growth of the norm of $(\delta p_i, \delta q_i)$. In fact, for the dynamics of a bound system this quantity obviously is bounded. But even then the exponent in (3.12) will often grow exponentially due to the presence of the stability matrices $S_t^0$ and $S_t^c$.

The contributions of $F_{\text{disp}}(t)$ and of $F_{\text{class}}(t)$ to the decay of fidelity will now be studied separately. This procedure makes sense if $\hbar$ simultaneously approaches zero in order to maintain the condition $t \ll T_E(\hbar)$. In this regime the individual contributions to $F(t)$ determine the leading behaviour of the fidelity as $t \to \infty$ and $\hbar \to 0$ completely.

### 3.1 Contribution of wave packet dispersion

We begin with discussing the behaviour of $F_{\text{disp}}(t)$ as $t \to \infty$. Since both $G_{S_t^0[Z]}$ and $G_{S_t^c[Z]}$ are symmetric and positive-definite, we can convert these matrices into a diagonal form as explained in Appendix B. This implies that there exists a real, invertible matrix $M_t$ such that $M_t^T G_{S_t^0[Z]} M_t = \mathbf{1}$, and at the same time $M_t^T G_{S_t^c[Z]} M_t = D_t$ is diagonal, with the (positive) eigenvalues $\Lambda_k(t)$ of

$$G_{S_t^0[Z]}^{-1} G_{S_t^c[Z]} = S_t^0 G_Z^{-1} ((S_t^c)^{-1} S_t^0)^T G_Z (S_t^c)^{-1}$$

(3.13) on the diagonal. Furthermore, since $G_Z$ is symmetric and positive-definite, it is a square of a symmetric and positive-definite matrix, $G_Z = \gamma^2$. Hence, (3.13) is conjugate to a matrix $N_t^T N_t$, with $N_t = \gamma (S_t^c)^{-1} S_t^0 \gamma^{-1}$. This means that the eigenvalues $\Lambda_k(t)$ of (3.13) are squares of the singular values $\mu_k(t)$ of $N_t$ (see Appendix C). Since $\gamma$ is independent of $t$ the time dependence of $\mu_k(t)$ therefore is asymptotically determined by the singular values $\tilde{\mu}_k(t)$ of $(S_t^c)^{-1} S_t^0$. More precisely, there exist constants $C_1, C_2 > 0$ such that

$$C_1 \tilde{\mu}_k(t) \leq \mu_k(t) \leq C_2 \tilde{\mu}_k(t) .$$

(3.14)

We also exploit the fact that the product $(S_t^c)^{-1} S_t^0$ of two symplectic matrices is again symplectic. This implies that its singular values $\tilde{\mu}_k(t)$ arise in pairs of mutually inverse numbers. Thus, they can be ordered as in (C.7).

The determinant that yields $F_{\text{disp}}(t)$ according to (3.11) can be evaluated as in Appendix B see (B.1). Taking into account that $G_{S_t^0[Z]}$ has unit determinant and that the eigenvalues $\Lambda_k(t)$ of (3.13) are given by squares of the singular values $\mu_k(t)$, we obtain

$$F_{\text{disp}}(t) = \left[ \prod_{k=1}^{2d} \left(1 + \mu_k(t)^2\right) \right]^{-1/2} .$$

(3.15)
The estimates (3.14) then allow to bound (3.15) from below and above in terms of
\[
\left[ \prod_{k=1}^{d} \left( \tilde{\mu}_k(t)^2 + 2 + \tilde{\mu}_k(t)^{-2} \right) \right]^{-1/2}.
\] (3.16)

More specifically, there exist constants \( C_3, C_4 > 0 \) such that
\[
C_3 \prod_{k=1}^{d} \tilde{\mu}_k(t)^{-1} \leq F_{\text{disp}}(t) \leq C_4 \prod_{k=1}^{d} \tilde{\mu}_k(t)^{-1}.
\] (3.17)

Since the product over the inverse singular values contains only factors with \( \tilde{\mu}_k(t) \geq 1 \), one can introduce the simple estimate
\[
\tilde{\mu}_{\text{max}}(t) \leq \prod_{k=1}^{d} \tilde{\mu}_k(t) \leq \tilde{\mu}_{\text{max}}(t)^{d-1} \tilde{\mu}_d(t).
\] (3.18)

The quantities \( \tilde{\mu}_k(t) \) are singular values of a product of two symplectic matrices to which the inequalities (C.8) may be applied. Thus, when choosing \( k = 1 \) in (C.8), the l.h.s. of (3.18) can be bounded from below by
\[
\max \left\{ \frac{\mu_{\text{max}}(S^0_t)}{\mu_{\text{max}}(S^\varepsilon_t)}, \frac{\mu_{\text{max}}(S^\varepsilon_t)}{\mu_{\text{max}}(S^0_t)} \right\} \leq \tilde{\mu}_{\text{max}}(t).
\] (3.19)

Furthermore, the maximal singular values of \( S^\varepsilon_t \) and \( S^0_t \) determine the maximal Lyapunov exponents according to
\[
\lambda^{0/\varepsilon} = \limsup_{t \to \infty} \frac{1}{t} \log \| S^{0/\varepsilon}_t \|_{\text{HS}}
\]
\[
= \limsup_{t \to \infty} \frac{1}{t} \log \mu_{\text{max}}(S^{0/\varepsilon}_t),
\] (3.20)

so that in case \( \delta \lambda = \lambda^\varepsilon - \lambda^0 \neq 0 \) the l.h.s. of (3.19) is asymptotic to \( e^{\delta \lambda t} \) as \( t \to \infty \).

The r.h.s. of (3.18) may now be estimated in a similar manner: Apply the rightmost inequality in (C.8) to each factor, and for the term with \( k = d \) use that \( \mu_d(S^{0/\varepsilon}_t) = 1 \), see Appendix C. This finally yields the upper bound
\[
\left[ \mu_{\text{max}}(S^0_t) \mu_{\text{max}}(S^\varepsilon_t) \right]^{d-1} \cdot \min \left\{ \mu_{\text{max}}(S^0_t), \mu_{\text{max}}(S^\varepsilon_t) \right\}
\] (3.21)

for \( \tilde{\mu}_{\text{max}}(t)^{d-1} \tilde{\mu}_d(t) \). Asymptotically, as \( t \to \infty \) this approaches \( \exp \left\{ \min \{ \lambda^0, \lambda^\varepsilon \} \right\} t \).

The above estimates can be summarised to provide the following statement about the asymptotic behaviour of \( F_{\text{disp}}(t) \): There exist constants \( C_5, C_6 > 0 \) such that
\[
C_5 e^{-Lt} \leq F_{\text{disp}}(t) \leq C_6 e^{-Lt},
\] (3.22)

with
\[
|\delta \lambda| \leq L \leq (d-1)(\lambda^0 + \lambda^\varepsilon) + \min \{ \lambda^0, \lambda^\varepsilon \}.
\] (3.23)

Thus, once the maximal Lyapunov exponent of the perturbed dynamics differs from the unperturbed one, the asymptotic decay of \( F_{\text{disp}}(t) \) is essentially exponential.
3.2 Contribution of classical trajectories

The remaining factor $F_{\text{class}}(t)$ that determines the decay of fidelity is influenced by the linear stabilities of the perturbed and of the unperturbed classical trajectories as well as by the separation $(\delta p_t, \delta q_t)$ of the trajectories. The contribution of the stabilities can be treated in a similar manner as above, whereas the behaviour of the separation is largely unknown in a general linearly unstable system. Precise estimates are rare, but can possibly be achieved in particular cases (see, e.g., Section 4 and [19]).

A first simplification of the expression (3.12) can be achieved by introducing the matrix $M_t$ that converts $G_s^0[Z]$ and $G_s^0[Z]$ into a diagonal form. The exponent of (3.12), without the factor $-1/\hbar$, then reads

$$M_t^{-1}(\delta p_t, \delta q_t) \cdot (1 - (1 + D_t)^{-1}) M_t^{-1}(\delta p_t, \delta q_t)$$

(3.24)

where, as above, $D_t = M_t^T G_s^0[Z] M_t$ is the diagonal matrix with the eigenvalues $\Lambda_k(t) > 0$ on its diagonal. The quadratic form $1 - (1 + D_t)^{-1}$ defined by (3.24) is positive-definite; its eigenvalues are $\Lambda_k(t)/(1 + \Lambda_k(t)) > 0$. Thus, whatever value the separation $(\delta p_t, \delta q_t)$ attains, one immediately concludes that $F_{\text{class}}(t) \leq 2^d$. And although the eigenvalues $\Lambda_k(t)$ may eventually grow as $t \to \infty$, this quadratic form remains bounded. Any influence of the linear stabilities on $F_{\text{class}}(t)$ hence is encoded in the matrices $M_t$ as they appear in (3.24).

An upper bound for the expression (3.24) follows from the estimate (C.9) derived in Appendix C when choosing $A = 1 - (1 + D_t)^{-1}$ and $B = M_t^{-1}$.

We notice that this is given by the sum of the eigenvalues $\Lambda_k(t)/(1 + \Lambda_k(t))$. These can be grouped in pairs with $\Lambda_k(t)$ and $\Lambda_k(t)^{-1}$ since the latter are eigenvalues of a symplectic matrix. Thus

$$\|A\|_{tr} = \sum_{k=1}^d \left( \frac{\Lambda_k(t)}{1 + \Lambda_k(t)} + \frac{\Lambda_k(t)^{-1}}{1 + \Lambda_k(t)^{-1}} \right) = d.$$  

(3.25)

Furthermore, we observe that

$$\|M_t^{-1}\|^2_{\text{HS}} = \text{tr}(M_t M_t^T)^{-1} = \|G_s^0[Z]\|_{tr}.$$  

(3.26)

Using (3.9), the rightmost expression can be factorised with the help of (C.4), leading to

$$\|M_t^{-1}\|^2_{\text{HS}} \leq \|S_t^0\|^2_{\text{HS}} \|G_Z\|_{\text{HS}}.$$  

(3.27)

Our final upper bound for (3.24) therefore reads

$$d \|G_Z\|_{\text{HS}} \|S_t^0\|^2_{\text{HS}} (\delta p_t^2 + \delta q_t^2).$$

(3.28)

For the contribution (3.12) to the fidelity this provides us with a lower bound of the form

$$F_{\text{class}}(t) \geq 2^d \exp \left[-\frac{d}{\hbar} \|G_Z\|_{\text{HS}} \|S_t^0\|^2_{\text{HS}} (\delta p_t^2 + \delta q_t^2)\right].$$

(3.29)

In addition, if the unperturbed trajectory possesses a positive maximal Lyapunov exponent, the factor $\|S_t^0\|^2_{\text{HS}}$ grows asymptotically like $e^{2\lambda \delta t}$, see (3.20).


In order to achieve a lower bound for (3.24) according to (C.10) we first notice that the symplecticity of (3.13) implies \( \Lambda_{\min}(t) = \Lambda_{\max}(t)^{-1} = \mu_{\max}(t)^{-2} \). This leads to
\[
\Lambda_{\min}(A) = \frac{1}{1 + \mu_{\max}(t)^2} \geq \frac{1}{2} \mu_{\max}(t)^{-2}.
\] (3.30)

Then (3.14) and (C.6) yield the further bound
\[
\Lambda_{\min}(A) \geq K_1 \mu_{\max}((S^e_t)^{-1}S^0_t)^{-2} \geq K_1 \mu_{\max}(S^e_t)^{-2} \mu_{\max}(S^0_t)^{-2}
\] (3.31)

with some constant \( K_1 > 0 \). We now require a lower bound for \( \mu_{2d}(B)^2 = \mu_{2d}(M_t^{-1})^2 \), and first notice that this quantity is the lowest eigenvalue of \( (M_tM_t^T)^{-1} = G_{S^0_t[Z]} \), which in turn is the inverse of the largest eigenvalue of this matrix. Making use of the relation (C.6) we then conclude that
\[
\Lambda_{\max}(G_{S^0_t[Z]}) = \mu_{\max}(((S^0_t)^{-1})^TG_Z(S^0_t)^{-1}) \leq \mu_{\max}(G_Z) \mu_{\max}(S^0_t)^2.
\] (3.32)

Collecting the above estimates therefore provides us with the lower bound
\[
K_2 \mu_{\max}(S^e_t)^{-2} \mu_{\max}(S^0_t)^{-4}(\delta p_i^2 + \delta q_i^2)
\] (3.33)

for (3.24), with some \( K_2 > 0 \). Hence,
\[
F_{\text{class}}(t) \leq 2^d \exp\left[-\frac{K_2}{\hbar} \frac{\delta p_i^2 + \delta q_i^2}{\mu_{\max}(S^e_t)^2 \mu_{\max}(S^0_t)^4}\right].
\] (3.34)

Furthermore, in the case of linearly unstable trajectories (3.20) implies that
\[
\mu_{\max}(S^e_t)^2 \mu_{\max}(S^0_t)^4 \sim \exp[(2\lambda^e + 4\lambda^0)t],
\] (3.35)

as \( t \to \infty \).

We have so far refrained from estimating the squared distance \( \delta p_i^2 + \delta q_i^2 \) the perturbed trajectory can separate itself away from the unperturbed one. However, any further statements about the decay of \( F_{\text{class}}(t) \) require some knowledge of the behaviour of that distance. But this, as already mentioned, seems to be difficult to obtain. E.g., one can in general not exclude that this quantity vanishes infinitely often (see [19] for a particular case), or asymptotically approaches zero. Such situations may occur, if the perturbation \( V(p, q) \) is confined to a bounded part of phase space, but the trajectories are forced to leave this domain in a particular channel. According to (3.12), at those instances where \( \delta p_i^2 + \delta q_i^2 \) vanishes, \( F_{\text{class}}(t) \) clearly acquires its maximal possible value \( 2^d \). On the other hand, if the energy shells corresponding to both the perturbed and the unperturbed classical Hamiltonians are bounded, \( \delta p_i^2 + \delta q_i^2 \) will necessarily be bounded, too.
However, if the classical motion is unbounded (as in the example in Section 4), an upper bound for this distance would be helpful. In order to achieve such an estimate we consider a Taylor expansion of \((p_\varepsilon, q_\varepsilon)\) about \(\varepsilon = 0\) with remainder term of first order, i.e.,

\[
(\delta p_\varepsilon, \delta q_\varepsilon) = -\theta \varepsilon \left. \frac{d}{d\varepsilon'} (p_{\varepsilon'}, q_{\varepsilon'}) \right|_{\varepsilon' = \theta \varepsilon},
\]

where \(\theta \in [0, 1]\). The derivative on the r.h.s. can now be identified as a solution of a differential equation in the variable \(t\). Abbreviating

\[
z_\varepsilon(t) = \frac{d}{d\varepsilon} (p_\varepsilon, q_\varepsilon),
\]

the fact that \((p_0, q_0) = (p, q)\) for all \(\varepsilon\) implies the initial condition \(z_\varepsilon(0) = 0\). Moreover, a derivative of Hamilton’s equations of motion

\[
(\dot{p}_\varepsilon, \dot{q}_\varepsilon) = J H'_\varepsilon(p_\varepsilon, q_\varepsilon)
\]

w.r.t. \(\varepsilon\) yields

\[
\dot{z}_\varepsilon(t) = J H''_\varepsilon(p_\varepsilon, q_\varepsilon) z_\varepsilon(t) + J V'(p_\varepsilon, q_\varepsilon),
\]

where \(V'(p, q)\) denotes the gradient of the function \(V(p, q)\) whose Weyl quantisation yields the perturbation \(\hat{V}\) of the quantum Hamiltonian. A solution of the inhomogeneous differential equation (3.39) with the prescribed initial condition is then provided by the integral

\[
z_\varepsilon(t) = S_t^\varepsilon \int_0^t (S_s^\varepsilon)^{-1} J V'(p_s^\varepsilon, q_s^\varepsilon) \, ds.
\]

Used on the r.h.s. of (3.36) this expression allows us to relate the separation \((\delta p_\varepsilon, \delta q_\varepsilon)\) of the trajectories to their linear stabilities and properties of the derivative of the classical perturbation \(V\).

A quantitative upper bound that immediately follows from (3.40) is

\[
0 \leq |(\delta p_\varepsilon, \delta q_\varepsilon)| \leq \varepsilon \theta t \|S_t^\varepsilon\|_{HS} \sup_{s \in [0, t]} \|S_s^\varepsilon\|_{HS} \frac{1}{t} \int_0^t |V'(p_s^\varepsilon, q_s^\varepsilon)| \, ds
\]

\[
\leq \varepsilon t \left(\Sigma^\varepsilon_t\right)^2 \sup_{\theta \in [0, 1]} \frac{1}{t} \int_0^t |V'(p_s^\varepsilon, q_s^\varepsilon)| \, ds.
\]

Here we have introduced

\[
\Sigma^\varepsilon_t = \sup_{s \in [0, t], \theta \in [0, 1]} \|S_s^\varepsilon\|_{HS},
\]

whose asymptotic behaviour in the case of linearly unstable trajectories is controlled by the exponent

\[
\lambda^\varepsilon = \sup_{\theta \in [0, 1]} \lambda^\theta \varepsilon.
\]
Furthermore, under favourable circumstances the time average $\overline{V}$ of $V'$ in (3.41) is finite as $t \to \infty$; then the asymptotic behaviour of the r.h.s. in (3.41) for large times is given by

$$\varepsilon \overline{V} t e^{2\lambda t}.$$  (3.44)

This will, e.g., be the case if either the trajectory remains in a bounded set, or the derivative $V'$ is a bounded function on the respective energy shell.

## 4 Inverted oscillators

We want to discuss a simple and exactly solvable example that nevertheless possesses the typical features of exponentially unstable classical dynamics: a $d$-dimensional inverted harmonic oscillator. In that case the Hamiltonian is quadratic in position and momentum and therefore the semiclassical propagation (2.7) is exact, i.e., the error term vanishes.

To be specific, let

$$H_0(p, q) = \frac{1}{2} p^2 - \frac{\omega^2}{2} q^2,$$  (4.1)

and define

$$H_\varepsilon(p, q) = H_0(p, q - \varepsilon a),$$  (4.2)

so that, up to a constant, $V(q) = \omega^2 a \cdot q$. This perturbation consists of a phase space translation of the unperturbed Hamiltonian and hence is of the same type as the one discussed in [20]. The equations of motion generated by the unperturbed and by the perturbed Hamiltonian, respectively, can be solved explicitly, leading to

$$p_0^t = p \cosh \omega t + q \omega \sinh \omega t,$$
$$q_0^t = q \cosh \omega t + p \omega^{-1} \sinh \omega t,$$  (4.3)

and

$$\delta p_t = a \varepsilon \omega \sinh \omega t,$$
$$\delta q_t = a \varepsilon (\cosh \omega t - 1).$$  (4.4)

From (2.10), (4.3), and (4.4) one, moreover, obtains

$$S^\varepsilon_t = S^0_t = \left( \begin{array}{cc} \cosh \omega t \mathbb{1} & \omega \sinh \omega t \mathbb{1} \\ \omega^{-1} \sinh \omega t \mathbb{1} & \cosh \omega t \mathbb{1} \end{array} \right).$$  (4.5)

This implies an accidental coincidence of the unperturbed and the perturbed Lyapunov exponents: $\lambda^0 = \omega = \lambda^\varepsilon$. Furthermore, $G_{S^\varepsilon_t[Z]} = G_{S^0_t[Z]}$ so that $F_{\text{disp}}(t) = 2^{-d}$, reflecting the fact that the coinciding perturbed and unperturbed linearised dynamics lead to the same dispersions of the wave packets. Since $\delta \lambda = 0$, this finding is in accordance with the bounds (3.23). With the help of the relation (A.8) and a change of variables the expression (3.3) for the fidelity can now be brought into the form

$$F(t) = \int\int W[\phi^h](\eta, y) - S_t^{-1}(\delta p_t, \delta q_t)) W[\phi^h](\eta, y) \frac{d\eta dy}{(2\pi \hbar)^d}.$$  (4.6)
Therefore, in this example the quantum fidelity is crucially determined by the separation (4.4) of the classical trajectories.

For simplicity one can imagine the initial wave packet to be a Gaussian (2.1) with $Z = i$ that is localised at the unstable fixed point $(p, q) = (0, 0)$ of the unperturbed classical dynamics. Thus, $(p^0, q^0) = (0, 0)$ for all $t$, so that the unperturbed time evolution (2.7) fixes the centre of the wave packet and only forces it to disperse according to the action of the metaplectic operator related to (4.5). The perturbed dynamics, however, pushes the centre away from the fixed point according to (4.4). This happens with an exponential rate that follows from the asymptotic behaviour

$$|⟨(δp_t, δq_t)| \sim \frac{ε|a|}{2} \sqrt{λ^2 + 1} e^{λt}, \quad t \to \infty,$$

(4.7)

of the distance, which may be compared with the corresponding asymptotics

$$ε|a|λ^2 t e^{2λt}$$

(4.8)

of the upper bound (3.41), see also (3.44).

For Gaussian states either (3.12) or (4.6) can be evaluated directly, yielding

$$F(t) = \exp\left[ -\frac{ε^2a^2}{2\hbar}((1 - \cosh λt)^2 - λ^2 \sinh^2 λt) \right].$$

(4.9)

In this example the quantum fidelity therefore decays extremely fast, namely in a double exponential manner. We stress that neither have approximations been performed nor have any assumptions entered, and hence the result holds unconditionally. Clearly, this finding is at variance with the previous predictions of an exponential decay of fidelity. However, it obviously complies with the bounds (3.29) and (3.34) derived in Section 3. We remark that the double exponential decay is caused by both the separation (4.4) of the trajectories and the exponential instability of the linearised dynamics (4.5). Each of these factors alone would lead to this effect.

## 5 Conclusions

Our approach to the quantum fidelity of localised wave packets led us to distinguish two effects that derive from two separate contributions to the semiclassical evolution prior to the Ehrenfest time.

One effect is caused by the dispersion of the wave packets, which semiclassically originates from the metaplectic representation of the linearised classical dynamics. Since generically the unperturbed and the perturbed classical dynamics possess different linearisations, the resulting non-coinciding dispersions cause an eventually exponential contribution $F_{\text{disp}}(t)$ to the decay of fidelity as described by (3.22) and (3.23).

A second effect is due to the separation of the perturbed classical trajectory away from the unperturbed one. Since the centres of the wave packets follow their associated classical
trajectories, this divergence forces the overlap of the unperturbed with the perturbed time evolution of the given initial state to decrease. We estimated this contribution, \( F_{\text{class}}(t) \), for Gaussian wave packets and identified an influence of the linear stabilities as well as of the separation of the trajectories. Since in general the latter cannot be well controlled, we were unable to determine a uniform expression for this factor. The bounds \((3.29), (3.34), \) and \((3.41)\) that we obtained allow for decays that are exponentially faster, or slower, than exponential. Of course, the further factor \( F_{\text{disp}}(t) \) always ensures that the fidelity decays at least exponentially.

In view of the previous predictions of an exponential fidelity decay a contribution that decreases in a double exponential manner might come as a surprise. In the example of inverted harmonic oscillators, however, we saw that such a behaviour is indeed possible. In that case this was caused by both the linear instability of the classical motion and by the exponentially growing separation of the trajectories. The latter effect is certainly not generic if one has chaotic systems with bounded energy shells in mind. Nevertheless, in our example the linear instability alone would cause a doubly exponentially decreasing factor. And this is in perfect agreement with the bound \((3.29)\) that applies in the general case, even if the separation of trajectories does not exceed a given bound.

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Appendices

A Metaplectic representation

In this appendix we collect some important facts about the symplectic group and the metaplectic representation. For further details see [15, 16, 17].

The symplectic group consists of the linear canonical transformations \((p, q) \mapsto (p', q')\) with

\[
\begin{align*}
p' &= Ap + Bq , \\
q' &= Cp + Dq .
\end{align*}
\]

(A.1)

The real \(2d \times 2d\) matrix

\[
S = \begin{pmatrix} A & B \\ C & D \end{pmatrix}
\]

(A.2)

then fulfills \(S^TJS = J\), where

\[
J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} , \quad J^2 = -I ,
\]

(A.3)
is the symplectic unit. The symplectic group is generated by the matrices

\[ S_A = \begin{pmatrix} A & 0 \\ 0 & (A^T)^{-1} \end{pmatrix}, \quad S_C = \begin{pmatrix} I & C \\ 0 & I \end{pmatrix}, \quad J, \]

(A.4)

where \( A \) is an invertible matrix and \( C \) is symmetric.

A quantisation of a linear canonical transformation \( (A.1) \) requires a unitary ray-representation of the symplectic group. This can be obtained from the observation that the operators \( \hat{D}(p,q) \) and \( \hat{D}((S^T)^{-1}(p,q)) \), see \( (2.4) \), each provide a unitary irreducible representation of the Heisenberg group. According to the Stone-Von Neumann Theorem there hence exists a unitary operator \( \hat{\mu}(S) \) such that

\[ \hat{D}((S^T)^{-1}(p,q)) = \hat{\mu}(S) \hat{D}(p,q) \hat{\mu}(S)^{-1}. \]

(A.5)

Choosing \( S = S_1S_2 \) furthermore implies the multiplicative property

\[ \hat{\mu}(S_1S_2) = e^{i\chi(S_1,S_2)} \hat{\mu}(S_1) \hat{\mu}(S_2). \]

(A.6)

In fact, the phase factor can be chosen to be \( \pm 1 \). The metaplectic operators \( \hat{\mu}(S) \) determine a double-valued representation of the symplectic group which is also known as the metaplectic representation.

Up to a sign the metaplectic representation is fixed once the metaplectic operators for the generators \( (A.4) \) are given. Exploiting the relation \( (A.5) \), one obtains

\[
\begin{align*}
\hat{\mu}(S_A)\psi(x) &= \sqrt{\det A} \psi(A^T x), \\
\hat{\mu}(S_C)\psi(x) &= \pm e^{\frac{i}{2}x^T C x} \psi(x), \\
\hat{\mu}(J)\psi(p) &= i^{d/2} \tilde{\psi}(p),
\end{align*}
\]

(A.7)

for them, where \( \tilde{\psi}(p) \) denotes the momentum representation of \( \psi \).

An explicit calculation based on the relation \( (A.5) \) finally reveals that the Wigner representation of a quantum state is covariant under linear canonical transformations,

\[ W[\hat{\mu}(S)\psi](\xi, x) = W[\psi](S^{-1}(\xi, x)). \]

(A.8)

Thus, if \( \psi \) is localised at the point \( (p, q) \) in phase space, the transformed state \( \hat{\mu}(S)\psi \) is concentrated at \( S(p, q) \).

B Diagonal form of positive matrices

It is well known that if two real and symmetric matrices commute, they can be simultaneously diagonalised by an orthogonal transformation. Less appreciated is the possibility of converting non-commuting, but positive-definite, symmetric matrices into a diagonal form with a single transformation:
Let $A$ and $B$ be real, symmetric, and positive-definite $n \times n$ matrices. Then there exists a real, invertible (not necessarily orthogonal) matrix $M$ such that $M^T AM = I$ and $M^T BM$ is diagonal, with the eigenvalues $\Lambda_j(A^{-1}B)$ of the positive-definite matrix $A^{-1}B$ on the diagonal. Moreover,

$$\det(A + B) = \prod_{j=1}^{n} \Lambda_j(A)[1 + \Lambda_j(A^{-1}B)] . \quad (B.1)$$

A proof of this statement is not difficult: Let $O$ be an orthogonal matrix such that $O^T AO = D$ is diagonal (and positive-definite). Define $U = OD^{-1/2}$, then $U^T AU = I$, and $U^T BU$ is symmetric and positive-definite. Furthermore, since $U^T BU = U^{-1}A^{-1}BU$, the matrices $U^T BU$ and $A^{-1}B$ have identical spectra. Hence there exists an orthogonal matrix $O_1$ such that $O_1^T U^T BU O_1$ is diagonal, with the eigenvalues $\Lambda_j(A^{-1}B)$ on the diagonal. Then define $M = UO_1$ to obtain the matrix $M$ of the statement.

\section*{C \hspace{1em} Matrix norms and singular values}

Real $n \times n$ matrices can be estimated in terms of various norms, for which there exists a number of inequalities that we want to review in this appendix. More details can, e.g., be found in [21].

The \textit{operator norm} is defined as

$$\|A\|_\text{op} = \sup_{\|x\| = 1} |A x| , \quad (C.1)$$

where $\|x\| = \sqrt{x^2}$ is the euclidean norm of a vector $x \in \mathbb{R}^n$. The \textit{trace norm}, however, is given by

$$\|A\|_\text{tr} = \text{tr} \sqrt{A^T A} . \quad (C.2)$$

Finally, we consider the \textit{Hilbert-Schmidt norm}

$$\|A\|_\text{HS} = \sqrt{\text{tr} A^T A} , \quad (C.3)$$

All of these matrix norms possess the multiplicative property $\|AB\| \leq \|A\|\|B\|$. Moreover, they fulfill

$$\|A\|_\text{op} \leq \|A\|_{\text{HS}} \leq \|A\|_\text{tr} ,$$

$$\|AB\|_\text{tr} \leq \|A\|_{\text{HS}}\|B\|_{\text{HS}} . \quad (C.4)$$

In addition, for symplectic matrices $S$ one obtains $\|S^{-1}\|_{\text{tr/HS}} = \|S\|_{\text{tr/HS}}$.

In general a real $n \times n$ matrix $A$ cannot be diagonalised. However, $A^T A$ is symmetric and positive-definite and therefore possesses $n$ non-negative eigenvalues. Their positive square-roots $\mu_j(A)$ are the \textit{singular values} of $A$, which we order as

$$\mu_{\max}(A) = \mu_1(A) \geq \mu_2(A) \geq \cdots \geq \mu_n(A) \geq 0 . \quad (C.5)$$
Furthermore, Fan’s inequality (see [21]) implies for the singular values of products that
\[ \mu_k(AB) \leq \mu_{\max}(A) \mu_k(B), \]
\[ \mu_k(AB) \leq \mu_{\max}(B) \mu_k(A). \]  \hfill (C.6)

The singular values of symplectic matrices occur in pairs of mutually inverse numbers. Since in that case \( n \) must be even, we write \( n = 2d \), and choose the following ordering:
\[ \mu_1(S) \geq \cdots \geq \mu_d(S) \geq \mu_{d}^{-1}(S) \geq \cdots \geq \mu_1^{-1}(S). \]  \hfill (C.7)

In addition to the upper bound (C.6), in the symplectic case one can also find a lower bound that is based on the fact that \( \mu_{\max}(S^{-1}) = \mu_{\max}(S) \). Choose first \( A = S_1S_2 \) and \( B = S_2^{-1} \), and then \( A = S_1^{-1} \) and \( B = S_1S_2 \) in (C.6). This results in
\[ \max \left\{ \frac{\mu_k(S_1)}{\mu_{\max}(S_2)}, \frac{\mu_k(S_2)}{\mu_{\max}(S_1)} \right\} \leq \mu_k(S_1S_2) \leq \min \left\{ \mu_k(S_1) \mu_{\max}(S_2), \mu_k(S_2) \mu_{\max}(S_1) \right\}. \]  \hfill (C.8)

In section 3.2 we need to estimate a quadratic form \( Bv \cdot ABv \) in terms of suitable norms of the positive-definite, symmetric matrix \( A \) and of the invertible matrix \( B \). An upper bound follows from the definition (C.1) of the operator norm and a subsequent application of (C.4),
\[ Bv \cdot ABv \leq \|A\|_{\text{op}} \|B\|_{\text{op}}^2 |v|^2 \]
\[ \leq \|A\|_{\text{tr}} \|B\|_{\text{HS}}^2 |v|^2. \]  \hfill (C.9)

A lower bound can be gained from the fact that the quadratic form defined by \( A \) attains its minimum at the eigenvector corresponding to the lowest eigenvalue \( \Lambda_{\min}(A) > 0 \). Thus
\[ Bv \cdot ABv \geq \Lambda_{\min}(A) |Bv|^2 \]
\[ = \Lambda_{\min}(A) v \cdot B^T Bv \]
\[ \geq \Lambda_{\min}(A) \mu_n(B)^2 |v|^2, \]  \hfill (C.10)

since by (C.5) \( \mu_n(B) \) is the lowest singular value of \( B \).

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