Stability of wave-packet dynamics under perturbations

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We introduce a method to investigate the stability of wave-packet dynamics under perturbations of the Hamiltonian. Our approach relies on semiclassical approximations, but is nonperturbative. 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 realized for inverted harmonic oscillators.

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I. 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 behavior of quantum time evolutions at large times has attracted an increasing attention (see, e.g., [3–6]). 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 behavior of quantum dynamics under a change of initial conditions one should investigate its stability under perturbations of the Hamiltonian. Suppose that an initial state ψ 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 ε is a variable parameter. Then the *quantum fidelity*

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

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) is also known as the *quantum Loschmidt echo*.

Peres analyzed $F(t)$ in perturbation theory, and found an initial decay $F(t) \sim 1 - C_{\hat{V},\psi}(\varepsilon t/\hbar)^2$, where $C_{\hat{V},\psi}$ is a constant that depends on the perturbation and on the initial state. 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 ε and $\hbar$. Later work focused on time scales beyond this perturbative regime or on strong perturbations, respectively, and found an exponential decay [8–11]. Its rate is determined either by Fermi's golden rule [8] or, for stronger perturbations, by a classical Lyapunov exponent [9,11]. Further studies related the behavior 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 such 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 nonperturbative (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 [9–11,13]. 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. 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. It may also be

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doubly exponential, which we show to be the case in the example of inverted harmonic oscillators.

This paper is organized as follows. In Sec. II 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 Sec. III, with an emphasis on the behavior of Gaussian states. An exact calculation of the fidelity for inverted harmonic oscillators is performed in Sec. IV. We finally summarize our findings in Sec. V. Three appendixes 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.

II. LOCALIZED WAVE PACKETS

The initial states to which our approach applies are wave packets with a localization 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 normalized, smooth, and rapidly decreasing functions $\phi(\boldsymbol{x})$ (Schwartz test functions) of $\boldsymbol{x}\in\mathbb{R}^d$. Examples for this are provided by the Gaussian functions

$$\phi^Z(\boldsymbol{x}) = \left(\frac{\det \operatorname{Im} Z}{\pi^d}\right)^{1/4} e^{(i/2)\boldsymbol{x}\cdot Z\boldsymbol{x}}, \tag{2}$$

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

$$\phi^\hbar(\boldsymbol{x}) = \hbar^{-d/4}\phi(\boldsymbol{x}/\sqrt{\hbar}). \tag{3}$$

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

$$W[\phi^\hbar](\boldsymbol{\xi},\boldsymbol{x}) = \int \overline{\phi^\hbar(\boldsymbol{x}-\boldsymbol{y}/2)}\,\phi^\hbar(\boldsymbol{x}+\boldsymbol{y}/2)e^{-(i/\hbar)\boldsymbol{y}\cdot\boldsymbol{\xi}}dy \tag{4}$$

which, if multiplied by $(2\pi\hbar)^{-d}$, converges to $\delta(\boldsymbol{\xi},\boldsymbol{x})$ as $\hbar\to 0$. A subsequent application of the phase space translation

$$\hat{D}(\boldsymbol{p},\boldsymbol{q}) = e^{-(i/\hbar)(\boldsymbol{q}\cdot\hat{\boldsymbol{P}}-\boldsymbol{p}\cdot\hat{\boldsymbol{Q}})} \tag{5}$$

therefore yields a wave packet

$$\phi^\hbar_{(\boldsymbol{p},\boldsymbol{q})}(\boldsymbol{x}) = e^{-(i/2\hbar)\boldsymbol{p}\cdot\boldsymbol{q}}\hat{D}(\boldsymbol{p},\boldsymbol{q})\phi^\hbar(\boldsymbol{x}) = e^{(i/\hbar)\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{q})}\phi^\hbar(\boldsymbol{x}-\boldsymbol{q}) \tag{6}$$

with phase space localization at the point $(\boldsymbol{p},\boldsymbol{q})$. 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 quantization of a classical Hamiltonian $H(\boldsymbol{p},\boldsymbol{q})$,

$$\hat{H}\psi(\boldsymbol{x}) = \iint H\left(\boldsymbol{p},\frac{\boldsymbol{x}+\boldsymbol{y}}{2}\right)e^{(i/\hbar)\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})}\psi(\boldsymbol{y})\frac{dp\,dy}{(2\pi\hbar)^d}, \tag{7}$$

can be determined semiclassically [3,14] to be

$$\hat{U}(t)\phi^\hbar_{(\boldsymbol{p},\boldsymbol{q})} = e^{(i/\hbar)R_t}\hat{D}(\boldsymbol{p}_t,\boldsymbol{q}_t)\hat{\mu}(S_t)\phi^\hbar + O_t(\sqrt{\hbar}). \tag{8}$$

The main term on the right-hand size (RHS) is again a wave packet of the type (6), but now localized at $(\boldsymbol{p}_t,\boldsymbol{q}_t)$. This is the point on the trajectory emerging in time t from the initial point $(\boldsymbol{p},\boldsymbol{q})$ under the classical dynamics generated by the Hamiltonian $H(\boldsymbol{p},\boldsymbol{q})$. Moreover,

$$R_t = \int_0^t [\dot{\boldsymbol{q}}_s\cdot\boldsymbol{p}_s - H(\boldsymbol{p}_s,\boldsymbol{q}_s)]ds \tag{9}$$

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

$$\dot{S}_t = JH''(\boldsymbol{p}_t,\boldsymbol{q}_t)S_t, \quad S_0 = \mathbb{1}. \tag{10}$$

Here J is the symplectic unit (A3) and $H''(\boldsymbol{p},\boldsymbol{q})$ is the Hessian matrix of the Hamiltonian. Equivalently, the stability matrix is given as

$$S_t = \begin{pmatrix} \dfrac{\partial\boldsymbol{p}_t}{\partial\boldsymbol{p}} & \dfrac{\partial\boldsymbol{p}_t}{\partial\boldsymbol{q}} \\ \dfrac{\partial\boldsymbol{q}_t}{\partial\boldsymbol{p}} & \dfrac{\partial\boldsymbol{q}_t}{\partial\boldsymbol{q}} \end{pmatrix}. \tag{11}$$

The wave packet at time t on the RHS of Eq. (8) arises from the initial state $\phi^\hbar$ 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 [15–17] for details. As can be drawn from (A8), a metaplectic operator does not change the semiclassical phase space localization. In (8) it is rather responsible for the dispersion of the wave packet. The second factor $D(\boldsymbol{p}_t,\boldsymbol{q}_t)$ 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 $(\boldsymbol{p}_t,\boldsymbol{q}_t)$. 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 $T_E(\hbar)=|\ln\hbar|/6\lambda$, the error term remains small. In contrast, if the trajectory is stable (in an integrable system or on a Kolmogorov-Arnold-Moser 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 (8) to infinite times, when $\hbar\to 0$. We remark that the main term in (8) actually is the leading contribution in a systematic semiclassical expansion [3]. If this is carried on to the Nth term, the error is $O_t(\hbar^{N/2})$ and can also be controlled up to $T_E(\hbar)$. At the Ehrenfest time the semiclassical representation (8) in terms of a single classical trajectory breaks down. Beyond this time scale a semiclassical time evolution requires considerably finer details of the classical phase space structures [6].

In order to determine the Wigner representation of the semiclassically leading term on the RHS of Eq. (8) one has to exploit the behavior of $W[\psi]$ for a quantum state ψ under phase space translations,

$$W[\hat{D}(\boldsymbol{p},\boldsymbol{q})\psi](\boldsymbol{\xi},\boldsymbol{x}) = W[\psi](\boldsymbol{\xi}-\boldsymbol{p},\boldsymbol{x}-\boldsymbol{q}), \tag{12}$$

and under metaplectic transformations; see (A8). This yields

$$W[\hat{D}(\boldsymbol{p}_t,\boldsymbol{q}_t)\hat{\mu}(S_t)\phi^{\hbar}](\boldsymbol{\xi},\boldsymbol{x}) = W[\phi^{\hbar}_{(\boldsymbol{p},\boldsymbol{q})}][(\boldsymbol{p},\boldsymbol{q}) + S_t^{-1}(\boldsymbol{\xi}-\boldsymbol{p}_t,\boldsymbol{x}-\boldsymbol{q}_t)]. \tag{13}$$

Hence, in phase space representation the leading semiclassical contribution to the time evolution of a wave packet, below the Ehrenfest time, is controlled by an approximate classical dynamics with trajectories

$$(\tilde{\boldsymbol{\xi}}_t,\tilde{\boldsymbol{x}}_t) = (\boldsymbol{p},\boldsymbol{q}) + S_t^{-1}(\boldsymbol{\xi}-\boldsymbol{p}_t,\boldsymbol{x}-\boldsymbol{q}_t). \tag{14}$$

Viewed as a map from $(\boldsymbol{\xi},\boldsymbol{x})$ to $(\tilde{\boldsymbol{\xi}}_t,\tilde{\boldsymbol{x}}_t)$, this is the inverse to the linearization of the full classical dynamics about the trajectory $(\boldsymbol{p}_t,\boldsymbol{q}_t)$. The trajectories (14) also occur when propagating observables in the Heisenberg picture in a semiclassical approximation corresponding to the RHS of Eq. (8); see [18].

III. FIDELITY DECAY

The quantum fidelity of an initial wave packet of the type (6) can most conveniently be calculated in the Wigner representation,

$$F(t) = |\langle \hat{U}_0(t)\phi^{\hbar}_{(\boldsymbol{p},\boldsymbol{q})}|\hat{U}_\varepsilon(t)\phi^{\hbar}_{(\boldsymbol{p},\boldsymbol{q})}\rangle|^2 = \iint W[\hat{U}_0(t)\phi^{\hbar}_{(\boldsymbol{p},\boldsymbol{q})}](\boldsymbol{\xi},\boldsymbol{x})W[\hat{U}_\varepsilon(t)\phi^{\hbar}_{(\boldsymbol{p},\boldsymbol{q})}](\boldsymbol{\xi},\boldsymbol{x})\frac{d\xi\, dx}{(2\pi\hbar)^d}. \tag{15}$$

We now introduce the semiclassical result (8) for the perturbed and for the unperturbed time evolution, respectively, to this expression. The corresponding unperturbed and perturbed classical trajectories will be denoted as $(\boldsymbol{p}_t^0,\boldsymbol{q}_t^0)$ and $(\boldsymbol{p}_t^\varepsilon,\boldsymbol{q}_t^\varepsilon)$. After using the relation (12) one may change variables and define $(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)=(\boldsymbol{p}_t^0-\boldsymbol{p}_t^\varepsilon,\boldsymbol{q}_t^0-\boldsymbol{q}_t^\varepsilon)$. For the leading semiclassical contribution to Eq. (15) one thus obtains

$$F_{\rm scl}(t) = \iint W[\hat{\mu}(S_t^0)\phi^{\hbar}](\boldsymbol{\xi}-\delta\boldsymbol{p}_t,\boldsymbol{x}-\delta\boldsymbol{q}_t) \times W[\hat{\mu}(S_t^\varepsilon)\phi^{\hbar}](\boldsymbol{\xi},\boldsymbol{x})\frac{d\xi\, dx}{(2\pi\hbar)^d}. \tag{16}$$

Since semiclassically the Wigner representations of localized wave packets, if divided by $(2\pi\hbar)^d$, approach δ functions, one obtains from Eq. (16) that the classical limit of the quantum fidelity is

$$\lim_{\hbar\to 0}\frac{F(t)}{(2\pi\hbar)^d} = \delta(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t), \tag{17}$$

when in this limit t is kept below the Ehrenfest time.

For a more detailed study of the expression (16) we now restrict ourselves to Gaussian initial states of the form (2) with the scaling (3). The action of a metaplectic operator on such states can be calculated explicitly [15–17],

$$\hat{\mu}(S)\phi^{Z,\hbar} = e^{i(\pi/2)\sigma}\phi^{S[Z],\hbar}. \tag{18}$$

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,

$$S[Z] = (AZ+B)(CZ+D)^{-1}, \quad S = \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{19}$$

Furthermore, σ is a Maslov phase defined through

$$e^{i(\pi/2)\sigma} = \left(\frac{\det \operatorname{Im} Z}{\det \operatorname{Im} S[Z]}\right)^{1/4}[\det(CZ+D)]^{-1/2}. \tag{20}$$

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

$$W[\phi^{Z,\hbar}](\boldsymbol{\xi},\boldsymbol{x}) = 2^d e^{-(1/\hbar)(\boldsymbol{\xi},\boldsymbol{x})\cdot G_Z(\boldsymbol{\xi},\boldsymbol{x})}, \tag{21}$$

where

$$G_Z = \begin{pmatrix} (\operatorname{Im} Z)^{-1} & -(\operatorname{Im} Z)^{-1}\operatorname{Re} Z \\ -\operatorname{Re} Z(\operatorname{Im} Z)^{-1} & \operatorname{Im} Z + \operatorname{Re} Z(\operatorname{Im} Z)^{-1}\operatorname{Re} Z \end{pmatrix} \tag{22}$$

is a symmetric, symplectic, and positive-definite $2d\times 2d$ matrix with unit determinant. The behavior of (22) under the transformation (19) can be inferred from an application of a metaplectic operator to a Gaussian state in the Wigner representation (21). This way, from Eqs. (18) and (A8) one concludes that

$$G_{S[Z]} = (S^{-1})^T G_Z S^{-1}. \tag{23}$$

Now, Eq. (16) is a Gaussian integral that can immediately be evaluated, and the result may be factorized according to

$$F_{\rm scl}(t) = F_{\rm disp}(t)F_{\rm class}(t). \tag{24}$$

The first factor

$$F_{\rm disp}(t) = [\det(G_{S_t^0[Z]} + G_{S_t^\varepsilon[Z]})]^{-1/2} \tag{25}$$

is determined by the dispersion of the wave packets. This interpretation follows from the fact that setting $\delta\boldsymbol{p}_t$ and $\delta\boldsymbol{q}_t$ to zero in Eq. (16), and therefore removing the phase space translations that arise from Eq. (8), the integral would exactly yield (25). In fact, $F_{\rm disp}(t)$ measures the differences in the dispersions caused by the two dynamics in question. This contribution is independent of $\hbar$. The time dependence of (25) follows from the relation (23) with S_t^0 and S_t^ε, 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 $F_{\rm class}(t)$ is influenced by the actual separation $(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)$ of these trajectories. It reads

$$F_{\text{class}}(t) = 2^d \exp\left(-\frac{1}{\hbar}(\delta \boldsymbol{p}_t, \delta \boldsymbol{q}_t) \cdot G_{S_t^0[Z]}(\mathbb{1} - \Gamma_{t,\varepsilon}^{-1})(\delta \boldsymbol{p}_t, \delta \boldsymbol{q}_t)\right),$$

$$\Gamma_{t,\varepsilon} = \mathbb{1} + G_{S_t^0[Z]}^{-1} G_{S_t^\varepsilon[Z]}, \tag{26}$$

and, despite its $\hbar$ dependence, essentially represents a classical fidelity in the sense of (17) since it is localized on the separation of the classical trajectories. This also explains the necessity of $\hbar$ in (26). We remark that expressions equivalent to (24)–(26) have independently been obtained by Combescure and Robert [19].

At this point we stress that in general the separation $(\delta \boldsymbol{p}_t, \delta \boldsymbol{q}_t)$ of the trajectories for large t differs essentially from the corresponding behavior of the linearized dynamics. In particular, an exponential instability expressed in terms of positive Lyapunov exponents does not imply an exponential growth of the norm of $(\delta \boldsymbol{p}_t, \delta \boldsymbol{q}_t)$. In fact, for the dynamics of a bound system this quantity obviously is bounded. But even then the exponent in Eq. (26) will often grow exponentially due to the presence of the stability matrices S_t^0 and S_t^ε.

An alternative view of the semiclassical fidelity for Gaussian wave packets is suggested by the fact that the Wigner representations (21) are positive. Hence, despite the presence of $\hbar$, one might be tempted to interpret them as classical phase space densities. In this context one would exploit the relation (13) to replace (16) with

$$F_{\text{scl}}(t) = \iint W[\phi_{(\boldsymbol{p},\boldsymbol{q})}^{Z,\hbar}](\tilde{\boldsymbol{\xi}}_t^0, \tilde{\boldsymbol{x}}_t^0) W[\phi_{(\boldsymbol{p},\boldsymbol{q})}^{Z,\hbar}](\tilde{\boldsymbol{\xi}}_t^\varepsilon, \tilde{\boldsymbol{x}}_t^\varepsilon) \frac{d\xi\, dx}{(2\pi\hbar)^d}. \tag{27}$$

If it were not for the appearance of $\hbar$ and of the approximate classical trajectories (14) instead of the actual ones, this expression would be the classical fidelity discussed in [20]. Due to the approximate (i.e., linearized) trajectories the quantity (27), however, is more closely related to the classical echoes studied in [21], when the diffusion constant is set to zero. Beyond the Ehrenfest time this analogy breaks down because then the semiclassical time evolution can no longer be based on single classical trajectories.

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 behavior of the fidelity as $t \to \infty$ and $\hbar \to 0$ completely.

A. Contribution of wave-packet dispersion

We begin with discussing the behavior of $F_{\text{disp}}(t)$ as $t \to \infty$. Since both $G_{S_t^0[Z]}$ and $G_{S_t^\varepsilon[Z]}$ 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 $M_t^T G_{S_t^0[Z]} M_t = \mathbb{1}$, and at the same time $M_t^T G_{S_t^\varepsilon[Z]} M_t = D_t$ is diagonal, with the (positive) eigenvalues $\Lambda_k(t)$ of

$$G_{S_t^0[Z]}^{-1} G_{S_t^\varepsilon[Z]} = S_t^0 G_Z^{-1} [(S_t^\varepsilon)^{-1} S_t^0]^T G_Z (S_t^\varepsilon)^{-1} \tag{28}$$

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, Eq. (28) is conjugate to a matrix $N_t^T N_t$, with $N_t = \gamma (S_t^\varepsilon)^{-1} S_t^0 \gamma^{-1}$. This means that the eigenvalues $\Lambda_k(t)$ of Eq. (28) are squares of the singular values $\mu_k(t)$ of N_t (see Appendix C). Since γ is independent of t the time dependence of $\mu_k(t)$ therefore is asymptotically determined by the singular values $\tilde{\mu}_k(t)$ of $(S_t^\varepsilon)^{-1} S_t^0$. More precisely, there exist constants $C_1, C_2 > 0$ such that

$$C_1 \tilde{\mu}_k(t) \leqslant \mu_k(t) \leqslant C_2 \tilde{\mu}_k(t). \tag{29}$$

We also exploit the fact that the product $(S_t^\varepsilon)^{-1} S_t^0$ 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 Eq. (C7).

The determinant that yields $F_{\text{disp}}(t)$ according to (25) can be evaluated as in Appendix B; see Eq. (B1). Taking into account that $G_{S_t^0[Z]}$ has unit determinant and that the eigenvalues $\Lambda_k(t)$ of Eq. (28) are given by squares of the singular values $\mu_k(t)$, we obtain

$$F_{\text{disp}}(t) = \left(\prod_{k=1}^{2d} [1 + \mu_k(t)^2]\right)^{-1/2}. \tag{30}$$

The estimates (29) then allow us to bound (30) from below and above in terms of

$$\left(\prod_{k=1}^{d} [\tilde{\mu}_k(t)^2 + 2 + \tilde{\mu}_k(t)^{-2}]\right)^{-1/2}. \tag{31}$$

More specifically, there exist constants $C_3, C_4 > 0$ such that

$$C_3 \prod_{k=1}^{d} \tilde{\mu}_k(t)^{-1} \leqslant F_{\text{disp}}(t) \leqslant C_4 \prod_{k=1}^{d} \tilde{\mu}_k(t)^{-1}. \tag{32}$$

Since the product over the inverse singular values contains only factors with $\tilde{\mu}_k(t) \geqslant 1$, one can introduce the simple estimate

$$\tilde{\mu}_{\max}(t) \leqslant \prod_{k=1}^{d} \tilde{\mu}_k(t) \leqslant \tilde{\mu}_{\max}(t)^{d-1} \tilde{\mu}_d(t). \tag{33}$$

The quantities $\tilde{\mu}_k(t)$ are singular values of a product of two symplectic matrices to which the inequalities (C8) may be applied. Thus, when choosing $k=1$ in (C8), the LHS of (33) can be bounded from below by

$$\max\left\{\frac{\mu_{\max}(S_t^0)}{\mu_{\max}(S_t^\varepsilon)}, \frac{\mu_{\max}(S_t^\varepsilon)}{\mu_{\max}(S_t^0)}\right\} \leqslant \tilde{\mu}_{\max}(t). \tag{34}$$

Furthermore, the maximal singular values of S_t^ε and S_t^0 determine the maximal Lyapunov exponents according to

$$\lambda^{0/\varepsilon} = \limsup_{t \to \infty} \frac{1}{t} \ln \| S_t^{0/\varepsilon} \|_{\text{HS}} = \limsup_{t \to \infty} \frac{1}{t} \ln \mu_{\max}(S_t^{0/\varepsilon}), \tag{35}$$

so that in case $\delta\lambda = \lambda^\varepsilon - \lambda^0 \neq 0$ the LHS of Eq. (34) is asymptotic to $e^{|\delta\lambda| t}$ as $t \to \infty$.

The RHS of Eq. (33) may now be estimated in a similar manner: Apply the rightmost inequality in (C8) to each factor, and for the term with $k=d$ use that $\mu_d(S_t^{0/\varepsilon}) = 1$ (see Appendix C). This finally yields the upper bound

$$[\mu_{\max}(S_t^0)\mu_{\max}(S_t^\varepsilon)]^{d-1}\min\{\mu_{\max}(S_t^0),\mu_{\max}(S_t^\varepsilon)\} \tag{36}$$

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

The above estimates can be summarized to provide the following statement about the asymptotic behavior of $F_{\rm disp}(t)$. There exist constants $C_5, C_6>0$ such that

$$C_5 e^{-Lt} \leqslant F_{\rm disp}(t) \leqslant C_6 e^{-Lt}, \tag{37}$$

with

$$|\delta\lambda| \leqslant L \leqslant (d-1)(\lambda^0+\lambda^\varepsilon)+\min\{\lambda^0,\lambda^\varepsilon\}. \tag{38}$$

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

B. Contribution of classical trajectories

The remaining factor $F_{\rm class}(t)$ 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 $(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)$ of the trajectories. The contribution of the stabilities can be treated in a similar manner as above, whereas the behavior 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., Sec. IV and [22]).

A first simplification of the expression (26) can be achieved by introducing the matrix M_t that converts $G_{S_t^0[Z]}$ and $G_{S_t^\varepsilon[Z]}$ into a diagonal form. The exponent of (26), without the factor $-1/\hbar$, then reads

$$M_t^{-1}(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)\cdot[\mathbb{1}-(\mathbb{1}+D_t)^{-1}]M_t^{-1}(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t), \tag{39}$$

where, as above, $D_t=M_t^T G_{S_t^\varepsilon[Z]}M_t$ is the diagonal matrix with the eigenvalues $\Lambda_k(t)>0$ on its diagonal. The quadratic form $\mathbb{1}-(\mathbb{1}+D_t)^{-1}$ defined by (39) is positive definite; its eigenvalues are $\Lambda_k(t)/[1+\Lambda_k(t)]>0$. Thus, whatever value the separation $(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)$ attains, one immediately concludes that $F_{\rm class}(t)\leqslant 2^d$. 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 $F_{\rm class}(t)$ hence is encoded in the matrices M_t as they appear in (39).

An upper bound for the expression (39) follows from the estimate (C9) derived in Appendix C when choosing $A=\mathbb{1}-(\mathbb{1}+D_t)^{-1}$ and $B=M_t^{-1}$. For the calculation of $\|A\|_{\rm tr}$ 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

$$\|A\|_{\rm tr}=\sum_{k=1}^{d}\left(\frac{\Lambda_k(t)}{1+\Lambda_k(t)}+\frac{\Lambda_k(t)^{-1}}{1+\Lambda_k(t)^{-1}}\right)=d. \tag{40}$$

Furthermore, we observe that

$$\|M_t^{-1}\|_{\rm HS}^2={\rm tr}(M_tM_t^T)^{-1}=\|G_{S_t^0[Z]}\|_{\rm tr}. \tag{41}$$

Using Eq. (23), the rightmost expression can be factorized with the help of (C4), leading to

$$\|M_t^{-1}\|_{\rm HS}^2 \leqslant \|S_t^0\|_{\rm HS}^2\|G_Z\|_{\rm HS}. \tag{42}$$

Our final upper bound for (39) therefore reads

$$d\|G_Z\|_{\rm HS}\|S_t^0\|_{\rm HS}^2(\delta\boldsymbol{p}_t^2+\delta\boldsymbol{q}_t^2). \tag{43}$$

For the contribution (26) to the fidelity this provides us with a lower bound of the form

$$F_{\rm class}(t)\geqslant 2^d\exp\left(-\frac{d}{\hbar}\|G_Z\|_{\rm HS}\|S_t^0\|_{\rm HS}^2(\delta\boldsymbol{p}_t^2+\delta\boldsymbol{q}_t^2)\right). \tag{44}$$

In addition, if the unperturbed trajectory possesses a positive maximal Lyapunov exponent, the factor $\|S_t^0\|_{\rm HS}^2$ grows asymptotically like $e^{2\lambda^0 t}$; see (35).

In order to achieve a lower bound for (39) according to (C10) we first notice that the symplecticity of (28) implies $\Lambda_{\min}(t)=\Lambda_{\max}(t)^{-1}=\mu_{\max}(t)^{-2}$. This leads to

$$\Lambda_{\min}(A)=\frac{1}{1+\mu_{\max}(t)^2}\geqslant\frac{1}{2}\mu_{\max}(t)^{-2}. \tag{45}$$

Then Eqs. (29) and (C6) yield the further bound

$$\Lambda_{\min}(A)\geqslant K_1\mu_{\max}[(S_t^\varepsilon)^{-1}S_t^0]^{-2}\geqslant K_1\mu_{\max}(S_t^\varepsilon)^{-2}\mu_{\max}(S_t^0)^{-2} \tag{46}$$

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 $(M_tM_t^T)^{-1}=G_{S_t^0[Z]}$, which in turn is the inverse of the largest eigenvalue of this matrix. Making use of the relation (C6) we then conclude that

$$\begin{aligned}\Lambda_{\max}(G_{S_t^0[Z]})&=\mu_{\max}\{[(S_t^0)^{-1}]^T G_Z(S_t^0)^{-1}\}\\&\leqslant\mu_{\max}(G_Z)\mu_{\max}(S_t^0)^2.\end{aligned} \tag{47}$$

Collecting the above estimates therefore provides us with the lower bound

$$K_2\mu_{\max}(S_t^\varepsilon)^{-2}\mu_{\max}(S_t^0)^{-4}(\delta\boldsymbol{p}_t^2+\delta\boldsymbol{q}_t^2) \tag{48}$$

for Eq. (39), with some $K_2>0$. Hence,

$$F_{\rm class}(t)\leqslant 2^d\exp\left(-\frac{K_2}{\hbar}\frac{\delta\boldsymbol{p}_t^2+\delta\boldsymbol{q}_t^2}{\mu_{\max}(S_t^\varepsilon)^2\mu_{\max}(S_t^0)^4}\right). \tag{49}$$

Furthermore, in the case of linearly unstable trajectories (35) implies that

$$\mu_{\max}(S_t^\varepsilon)^2\mu_{\max}(S_t^0)^4\sim\exp[(2\lambda^\varepsilon+4\lambda^0)t] \tag{50}$$

as $t\to\infty$.

We have so far refrained from estimating the squared distance $\delta\boldsymbol{p}_t^2+\delta\boldsymbol{q}_t^2$ the perturbed trajectory can separate itself away from the unperturbed one. However, any further statements about the decay of $F_{\rm class}(t)$ require some knowledge of the behavior of that distance. As already mentioned, this seems to be difficult to be obtained. For example, one can in general not exclude that this quantity vanishes infinitely often (see [22] for a particular case), or asymptotically approaches zero. Such situations may occur, if the perturbation $V(\boldsymbol{p},\boldsymbol{q})$ is confined to a bounded part of phase space, but the trajectories are forced to leave this domain in a particular channel. According to Eq. (26), at those instances where $\delta\boldsymbol{p}_t^2+\delta\boldsymbol{q}_t^2$ 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, $\delta\boldsymbol{p}_t^2+\delta\boldsymbol{q}_t^2$ will necessarily be bounded, too.

However, if the classical motion is unbounded (as in the example in Sec. IV), an upper bound for this distance would be helpful. In order to achieve such an estimate we consider a Taylor expansion of $(\boldsymbol{p}_t^\varepsilon,\boldsymbol{q}_t^\varepsilon)$ about $\varepsilon=0$ with remainder term of first order, i.e.,

$$(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t) = -\theta\varepsilon \frac{d}{d\varepsilon'}(\boldsymbol{p}_t^{\varepsilon'},\boldsymbol{q}_t^{\varepsilon'})\bigg|_{\varepsilon'=\theta\varepsilon}, \tag{51}$$

where $\theta\in[0,1]$. The derivative on the RHS can now be identified as a solution of a differential equation in the variable t. Abbreviating

$$z_\varepsilon(t) = \frac{d}{d\varepsilon}(\boldsymbol{p}_t^\varepsilon,\boldsymbol{q}_t^\varepsilon), \tag{52}$$

the fact that $(\boldsymbol{p}_0^\varepsilon,\boldsymbol{q}_0^\varepsilon)=(\boldsymbol{p},\boldsymbol{q})$ for all ε implies the initial condition $z_\varepsilon(0)=0$. Moreover, a derivative of Hamilton's equations of motion

$$(\dot{\boldsymbol{p}}_t^\varepsilon,\dot{\boldsymbol{q}}_t^\varepsilon) = JH_\varepsilon'(\boldsymbol{p}_t^\varepsilon,\boldsymbol{q}_t^\varepsilon) \tag{53}$$

with respect to ε yields

$$\dot{z}_\varepsilon(t) = JH_\varepsilon''(\boldsymbol{p}_t^\varepsilon,\boldsymbol{q}_t^\varepsilon)z_\varepsilon(t) + JV'(\boldsymbol{p}_t^\varepsilon,\boldsymbol{q}_t^\varepsilon), \tag{54}$$

where $V'(\boldsymbol{p},\boldsymbol{q})$ denotes the gradient of the function $V(\boldsymbol{p},\boldsymbol{q})$ whose Weyl quantization yields the perturbation $\hat{V}$ of the quantum Hamiltonian. A solution of the inhomogeneous differential equation (54) with the prescribed initial condition is then provided by the integral

$$z_\varepsilon(t) = S_t^\varepsilon\int_0^t (S_s^\varepsilon)^{-1}JV'(\boldsymbol{p}_s^\varepsilon,\boldsymbol{q}_s^\varepsilon)ds. \tag{55}$$

Used on the RHS of Eq. (51) this expression allows us to relate the separation $(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)$ 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 Eq. (55) is

$$0 \leqslant |(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)| \leqslant \varepsilon\theta t\|S_t^{\theta\varepsilon}\|_{\text{HS}} \sup_{s\in[0,t]}\|S_s^{\theta\varepsilon}\|_{\text{HS}}\frac{1}{t}\int_0^t |V'(\boldsymbol{p}_s^{\theta\varepsilon},\boldsymbol{q}_s^{\theta\varepsilon})|ds$$

$$\leqslant \varepsilon t(\Sigma_t^\varepsilon)^2 \sup_{\theta\in[0,1]}\frac{1}{t}\int_0^t |V'(\boldsymbol{p}_s^{\theta\varepsilon},\boldsymbol{q}_s^{\theta\varepsilon})|ds. \tag{56}$$

Here we have introduced

$$\Sigma_t^\varepsilon = \sup_{s\in[0,t],\theta\in[0,1]}\|S_s^{\theta\varepsilon}\|_{\text{HS}}, \tag{57}$$

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

$$\bar{\lambda}^\varepsilon = \sup_{\theta\in[0,1]}\lambda^{\theta\varepsilon}. \tag{58}$$

Furthermore, under favorable circumstances the time average $\bar{V}'$ of V' in (56) is finite as $t\to\infty$; then the asymptotic behavior of the RHS in (56) for large times is given by

$$\varepsilon\overline{V'}te^{2\bar{\lambda}^\varepsilon t}. \tag{59}$$

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.

IV. 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 (8) is exact, i.e., the error term vanishes.

To be specific, let

$$H_0(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{2}\boldsymbol{p}^2 - \frac{\omega^2}{2}\boldsymbol{q}^2, \tag{60}$$

and define

$$H_\varepsilon(\boldsymbol{p},\boldsymbol{q}) = H_0(\boldsymbol{p},\boldsymbol{q}-\varepsilon\boldsymbol{a}), \tag{61}$$

so that, up to a constant, $V(\boldsymbol{q})=\omega^2\boldsymbol{a}\cdot\boldsymbol{q}$. This perturbation consists of a phase space translation of the unperturbed Hamiltonian and hence is of the same type as the one discussed in [23]. The equations of motion generated by the unperturbed and by the perturbed Hamiltonian, respectively, can be solved explicitly, leading to

$$\boldsymbol{p}_t^0 = \boldsymbol{p}\cosh\omega t + \boldsymbol{q}\omega\sinh\omega t,$$

$$\boldsymbol{q}_t^0 = \boldsymbol{q}\cosh\omega t + \boldsymbol{p}\omega^{-1}\sinh\omega t, \tag{62}$$

and

$$\delta\boldsymbol{p}_t = \boldsymbol{a}\varepsilon\omega\sinh\omega t, \quad \delta\boldsymbol{q}_t = \boldsymbol{a}\varepsilon(\cosh\omega t - 1). \tag{63}$$

From Eqs. (11), (62), and (63) one, moreover, obtains

$$S_t^\varepsilon = S_t^0 = \begin{pmatrix} \cosh\omega t\mathbb{1} & \omega\sinh\omega t\mathbb{1} \\ \omega^{-1}\sinh\omega t\mathbb{1} & \cosh\omega t\mathbb{1}\end{pmatrix}. \tag{64}$$

This implies an accidental coincidence of the unperturbed and the perturbed Lyapunov exponents: $\lambda^0=\omega=\lambda^\varepsilon$. Furthermore, $G_{S_t^0[Z]}=G_{S_t^\varepsilon[Z]}$ so that $F_{\text{disp}}(t)=2^{-d}$, reflecting the fact that the coinciding perturbed and unperturbed linearized dynamics lead to the same dispersions of the wave packets. Since $\delta\lambda=0$, this finding is in accordance with the bounds (38). With the help of the relation (A8) and a change of variables the expression (16) for the fidelity can now be brought into the form

$$F(t)=\int\int W[\phi^{\hbar}][(\boldsymbol{\eta},\boldsymbol{y})-S_t^{-1}(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)]W[\phi^{\hbar}](\boldsymbol{\eta},\boldsymbol{y})\frac{d\eta\,dy}{(2\pi\eta)^d}. \tag{65}$$

Therefore, in this example the quantum fidelity is crucially determined by both the linear stability (64) and the separation (63) of the classical trajectories.

For simplicity one can imagine the initial wave packet to be a Gaussian (2) with $Z=i\mathbb{1}$ that is localized at the unstable fixed point $(\boldsymbol{p},\boldsymbol{q})=(0,0)$ of the unperturbed classical dynamics. Thus, $(\boldsymbol{p}_t^0,\boldsymbol{q}_t^0)=(0,0)$ for all t, so that the unperturbed time evolution (8) fixes the center of the wave packet and only forces it to disperse according to the action of the metaplectic operator related to (64). The perturbed dynamics, however, pushes the center away from the fixed point according to (63). This happens with an exponential rate that follows from the asymptotic behavior

$$|(\delta\boldsymbol{p}_t,\delta\boldsymbol{q}_t)|\sim\frac{\varepsilon|\boldsymbol{a}|}{2}\sqrt{\lambda^2+1}e^{\lambda t},\quad t\to\infty, \tag{66}$$

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

$$\varepsilon|\boldsymbol{a}|\lambda^2 te^{2\lambda t} \tag{67}$$

of the upper bound (56); see also (59).

For Gaussian states either (26) or (65) can be evaluated directly, yielding

$$F(t)=\exp\left(-\frac{\varepsilon^2\boldsymbol{a}^2}{2\hbar}[(1-\cosh\lambda t)^2+\lambda^2\sinh^2\lambda t]\right). \tag{68}$$

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 (44) and (49) derived in Sec. III. We remark that the double exponential decay is caused by both the separation (63) of the trajectories and the exponential instability of the linearized dynamics (64) which combine to produce the exponent in (68). Each of these contributions alone would lead to such a decay.

V. CONCLUSIONS

Our approach to the quantum fidelity of localized 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 linearized classical dynamics. Since generically the unperturbed and the perturbed classical dynamics possess different linearizations, the resulting noncoinciding dispersions cause an eventually exponential contribution $F_{\text{disp}}(t)$ to the decay of fidelity as described by Eqs. (37) and (38).

A second effect is due to the separation of the perturbed classical trajectory away from the unperturbed one. Since the centers 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 (44), (49), and (56) 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 behavior 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 (44) that applies in the general case, even if the separation of trajectories does not exceed a given bound.

Finally, we would like to take the opportunity of having the completely explicit result (68) for inverted oscillators available to discuss the restriction to times below the Ehrenfest time that we had to impose in our previous semiclassical studies of the fidelity. Since for large times the exponent in (68) behaves as $\text{const}\times(\varepsilon^2/\hbar)e^{2\lambda t}$, at $t=T_E(\hbar)=|\ln\hbar|/6\lambda$ it is of the order $\varepsilon^2\hbar^{-4/3}$. Hence, in order that (68) deviates appreciably from one before the Ehrenfest time the strength of the perturbation must satisfy the condition $\varepsilon\gg\hbar^{2/3}$. This may become relevant if one treats the perturbation of the dynamics in either quantum or classical perturbation theory. Thus, although the restriction to times below $T_E(\hbar)$ is not necessary in this example, this discussion shows that the characteristic decay of fidelity sets in prior to the Ehrenfest time once the perturbation does not become too small in the semiclassical limit. This is in particular true in our nonperturbative approach in which ε is fixed.

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APPENDIX A: METAPLECTIC REPRESENTATION

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

The *symplectic group* consists of the linear canonical transformations $(\boldsymbol{p},\boldsymbol{q})\mapsto(\boldsymbol{p}',\boldsymbol{q}')$ with

$$\boldsymbol{p}' = A\boldsymbol{p} + B\boldsymbol{q}, \quad \boldsymbol{q}' = C\boldsymbol{p} + D\boldsymbol{q}. \tag{A1}$$

The real $2d \times 2d$ matrix

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{A2}$$

then fulfills $S^T J S = J$, where

$$J = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \quad J^2 = -\mathbb{1}, \tag{A3}$$

is the symplectic unit. The symplectic group is generated by the matrices

$$S_A = \begin{pmatrix} A & 0 \\ 0 & (A^T)^{-1} \end{pmatrix}, \quad S_C = \begin{pmatrix} \mathbb{1} & C \\ 0 & \mathbb{1} \end{pmatrix}, \quad J, \tag{A4}$$

where A is an invertible matrix and C is symmetric.

A quantization of a linear canonical transformation (A1) requires a unitary ray representation of the symplectic group. This can be obtained from the observation that the operators $\hat{D}(\boldsymbol{p},\boldsymbol{q})$ and $\hat{D}[(S^T)^{-1}(\boldsymbol{p},\boldsymbol{q})]$ [see Eq. (5)] 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

$$\hat{D}[(S^T)^{-1}(\boldsymbol{p},\boldsymbol{q})] = \hat{\mu}(S)\hat{D}(\boldsymbol{p},\boldsymbol{q})\hat{\mu}(S)^{-1}. \tag{A5}$$

Choosing $S = S_1 S_2$ furthermore implies the multiplicative property

$$\hat{\mu}(S_1 S_2) = e^{i\chi(S_1,S_2)}\hat{\mu}(S_1)\hat{\mu}(S_2). \tag{A6}$$

In fact, the phase factor can be chosen to be ± 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 (A4) are given. Exploiting the relation (A5), one obtains

$$\hat{\mu}(S_A)\psi(\boldsymbol{x}) = \sqrt{\det A}\,\psi(A^T\boldsymbol{x}),$$

$$\hat{\mu}(S_C)\psi(\boldsymbol{x}) = \pm e^{(i/2\hbar)\boldsymbol{x}\cdot C\boldsymbol{x}}\psi(\boldsymbol{x}),$$

$$\hat{\mu}(J)\psi(\boldsymbol{p}) = i^{d/2}\hat{\psi}(\boldsymbol{p}) \tag{A7}$$

for them, where $\hat{\psi}(\boldsymbol{p})$ denotes the momentum representation of ψ.

An explicit calculation based on the relation (A5) finally reveals that the Wigner representation of a quantum state is covariant under linear canonical transformations,

$$W[\hat{\mu}(S)\psi](\boldsymbol{\xi},\boldsymbol{x}) = W[\psi][S^{-1}(\boldsymbol{\xi},\boldsymbol{x})]. \tag{A8}$$

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

APPENDIX B: DIAGONAL FORM OF POSITIVE MATRICES

It is well known that if two real and symmetric matrices commute, they can be simultaneously diagonalized by an orthogonal transformation. Less appreciated is the possibility of converting noncommuting, 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 $M^TAM = \mathbb{1}$ and M^TBM is diagonal, with the eigenvalues $\Lambda_j(A^{-1}B)$ of the positive definite matrix $A^{-1}B$ on the diagonal. Moreover,

$$\det(A+B) = \prod_{j=1}^{n} \Lambda_j(A)[1 + \Lambda_j(A^{-1}B)]. \tag{B1}$$

A proof of this statement is not difficult. Let O be an orthogonal matrix such that $O^TAO = D$ is diagonal (and positive definite). Define $U = OD^{-1/2}$; then $U^TAU = \mathbb{1}$, and U^TBU is symmetric and positive definite. Furthermore, since $U^TBU = U^{-1}A^{-1}BU$, the matrices U^TBU and $A^{-1}B$ have identical spectra. Hence there exists an orthogonal matrix O_1 such that $O_1^TU^TBUO_1$ 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.

APPENDIX C: 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 [24].

The *operator norm* is defined as

$$\|A\|_{\text{op}} = \sup_{|\boldsymbol{x}|=1} |A\boldsymbol{x}|, \tag{C1}$$

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

$$\|A\|_{\text{tr}} = \text{tr}\sqrt{A^TA}. \tag{C2}$$

Finally, we consider the *Hilbert-Schmidt norm*

$$\|A\|_{\text{HS}} = \sqrt{\text{tr}A^TA}. \tag{C3}$$

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

$$\|A\|_{\text{op}} \leq \|A\|_{\text{HS}} \leq \|A\|_{\text{tr}}, \quad \|AB\|_{\text{tr}} \leq \|A\|_{\text{HS}}\|B\|_{\text{HS}}. \tag{C4}$$

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 diagonalized. However, A^TA is symmetric and positive definite and therefore possesses n non-negative eigenvalues. Their positive square roots $\mu_j(A)$ are the *singular values* of A, which we order as

$$\mu_{\max}(A) = \mu_1(A) \geq \mu_2(A) \geq \cdots \geq \mu_n(A) \geq 0. \tag{C5}$$

Furthermore, Fan's inequality (see [24]) implies for the singular values of products that

$$\mu_k(AB) \leq \mu_{\max}(A)\mu_k(B),$$

$$\mu_k(AB) \leqslant \mu_{\max}(B)\mu_k(A). \tag{C6}$$

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:

$$\mu_1(S) \geqslant \cdots \geqslant \mu_d(S) \geqslant \mu_d(S)^{-1} \geqslant \cdots \geqslant \mu_1(S)^{-1}. \tag{C7}$$

In addition to the upper bound (C6), 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 (C6). This results in

$$\begin{aligned}\max\left\{\frac{\mu_k(S_1)}{\mu_{\max}(S_2)},\frac{\mu_k(S_2)}{\mu_{\max}(S_1)}\right\} &\leqslant \mu_k(S_1S_2)\\ &\leqslant \min\{\mu_k(S_1)\mu_{\max}(S_2),\mu_k(S_2)\mu_{\max}(S_1)\}. \end{aligned}\tag{C8}$$

In Sec. III B we need to estimate a quadratic form $B\boldsymbol{v}\cdot AB\boldsymbol{v}$ 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 (C1) of the operator norm and a subsequent application of (C4),

$$B\boldsymbol{v}\cdot AB\boldsymbol{v} \leqslant \|A\|_{\mathrm{op}}\|B\|_{\mathrm{op}}^2|\boldsymbol{v}|^2 \leqslant \|A\|_{\mathrm{tr}}\|B\|_{\mathrm{HS}}^2|\boldsymbol{v}|^2. \tag{C9}$$

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

$$\begin{aligned}B\boldsymbol{v}\cdot AB\boldsymbol{v} &\geqslant \Lambda_{\min}(A)|B\boldsymbol{v}|^2 = \Lambda_{\min}(A)\boldsymbol{v}\cdot B^TB\boldsymbol{v}\\ &\geqslant \Lambda_{\min}(A)\mu_n(B)^2|\boldsymbol{v}|^2,\end{aligned}\tag{C10}$$

since by Eq. (C5) $\mu_n(B)$ is the lowest singular value of B.

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