Symplectic Coarse-Grained Classical and Semiclassical Evolution of Subsystems: New Theoretical Aspects

Maurice A. de Gosson
University of Vienna
Faculty of Mathematics (NuHAG)
Oskar-Morgenstern-Platz 1
1090 Vienna AUSTRIA

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Abstract

We study the classical and semiclassical time evolutions of subsystems of a Hamiltonian system; this is done using a generalization of Heller’s thawed Gaussian approximation introduced by Littlejohn. The key tool in our study is an extension of Gromov’s ”principle of the symplectic camel”. This extension says that the orthogonal projection of a symplectic phase space ball on a phase space with a smaller dimension also contains a symplectic ball with the same radius. In the quantum case, the radii of these symplectic balls are taken equal to $\sqrt{\hbar}$ and represent ellipsoids of minimum uncertainty, which we have called ”quantum blobs” in previous work.

Introduction

Let us consider a bipartite physical system $A \cup B$ consisting of two subsystems $A$ and $B$ with phase spaces $\mathbb{R}^{2n_A}$ and $\mathbb{R}^{2n_B}$. We assume that both $A$ and $B$ are Hamiltonian, with respective Hamiltonian functions $H_A(x_A, p_A)$ and $H_B(x_B, p_B)$. As long as $A$ and $B$ do not interact in any way, the time evolution of the total system $A \cup B$ can be predicted by solving separately

* maurice.de.gosson@univie.ac.at
the Hamilton equations
\[
\begin{aligned}
\dot{x}_A &= \nabla_{p_A} H_A(x_A, p_A) \\
\dot{p}_A &= -\nabla_{x_A} H_A(x_A, p_A)
\end{aligned}
\] (1)

for the system \(A\) and those,
\[
\begin{aligned}
\dot{x}_B &= \nabla_{p_B} H_B(x_B, p_B) \\
\dot{p}_B &= -\nabla_{x_B} H_B(x_B, p_B)
\end{aligned}
\] (2)

for the system \(B\). The composite system \(A \cup B\) has Hamiltonian \(H = H_A + H_B\) defined on \(\mathbb{R}^{2n} \equiv \mathbb{R}^{2n_A} \times \mathbb{R}^{2n_B}\) and its evolution is fully determined by the values of \((x_A, p_A)\) and \((x_B, p_B)\) at some initial time, say, \(t = 0\). The situation becomes much more intricate when the two systems \(A\) and \(B\) are allowed to interact (which is generically the case). One must then add an interaction term \(H_{\text{inter}}\) to \(H_A + H_B\), and the total Hamiltonian is then
\[
H = H_A(x_A, p_A) + H_B(x_B, p_B) + H_{\text{inter}}(x_A, x_B; p_A, p_B). \tag{3}
\]

Such Hamiltonian functions frequently appear in molecular dynamics and in the Kepler problem. For instance, we can assume that the whole system consists of \(N\) molecules moving in physical three-dimensional space so that the full phase space is \(\mathbb{R}^{2n}\) with \(n = 3N\), and focus on a subset of \(N_A\) particles with phase space \(\mathbb{R}^{2n_A}, n_A = 3N_A\). This subset is then viewed as a classical open system [7, 8, 12] interacting with its environment. The solutions to Hamilton’s equations for (3) are generally in no way simply related to the solutions (1) and (2) of the uncoupled problem (1)–(2), making their study usually very complicated. For instance, let \(z_{A,0} = (x_{A,0}, p_{A,0})\) be an initial condition in \(\mathbb{R}^{2n_A}\) for the equations (1); this point is the projection of \(z_0 = (z_{A,0}, z_{B,0})\) for any values of \(z_{B,0} = (x_{B,0}, p_{B,0})\). The point \(z_0\), taken as initial datum for the Hamilton equations for \(H\), will in general be projected to infinitely many bifurcating trajectories in \(\mathbb{R}^{2n_A}\) all starting from \(z_{A,0}\); the solutions to the equations (1) will depend not only on the initial value \(z_{A,0}\) but are parametrized by those, \(z_{B,0}\), of the system \(B\); any change in the system \(B\) will affect the system \(A\). The motion of a subsystem of a Hamiltonian system is thus usually not Hamiltonian as soon as there are interactions with its environment. The situation is similar in quantum mechanics. In this case the Hamiltonian functions \(H_A\) and \(H_B\) are replaced with their quantizations \(\hat{H}_A = H_A(x_A, p_A), \hat{H}_B = H_B(x_B, p_B)\)

\[1\] The choice of a quantization scheme is always somewhat arbitrary; to keep things simple we will only use in this paper the usual Weyl quantization. This has many technical

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and the Hamilton equations (1) and (2) are replaced with the corresponding Schrödinger equations

\[ i\hbar \partial_t \psi_A = \hat{H}_A \psi_A , \quad \psi_A(\cdot, 0) = \psi_{A,0} \]  
\[ i\hbar \partial_t \psi_B = \hat{H}_B \psi_B , \quad \psi_B(\cdot, 0) = \psi_{B,0} \]  

where \( \psi_A \in L^2(\mathbb{R}^{n_A}) \) and \( \psi_B \in L^2(\mathbb{R}^{n_B}) \) describe the states of the quantized systems \( A \) and \( B \) at time \( t \). As long as the subsystems \( A \) and \( B \) do not interact, the evolution of the bipartite system \( A \cup B \) is determined by the Schrödinger equation

\[ i\hbar \partial_t \psi = (\hat{H}_A + \hat{H}_B) \psi , \quad \psi_{0} = \psi_{A,0} \otimes \psi_{B,0} . \]  

However, when \( A \) and \( B \) are allowed to interact, the evolution of \( A \cup B \) is described by the complete Schrödinger equation

\[ i\hbar \partial_t \psi = \hat{H} \psi , \quad \psi(\cdot, 0) = \psi_{0} \]  

where the operator

\[ \hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{\text{inter}} \]

is the quantization of the total Hamiltonian \( \h \) and \( \psi_{0} \in L^2(\mathbb{R}^n) \). Even when the initial wave function \( \psi_{0} \) is a tensor product \( \psi_{A,0} \otimes \psi_{B,0} \) the solution \( \psi \) at time \( t \) will generally not be a tensor product, because the state \( |\psi\rangle \) will be entangled [49, 53] and of the type

\[ \psi = \sum_j c_j \psi_{A,j} \otimes \psi_{B,j} \]

so it does not make sense to attribute to the subsystem \( A \) a pure state; it will rather evolve into a mixed state.

Let us briefly describe the strategy we will adopt to study the classical and quantum motion of subsystems. We begin by coarse-graining the total phase space \( \mathbb{R}^{2n} \) by balls \( B_{R}^{2n}(z_0) \) with small radius \( R \) and center \( z_0 \). The shadow (= orthogonal projection) of this ball on the phase space \( \mathbb{R}^{2n,A} \) of the subsystem \( A \) is of course a ball \( B_{R}^{2n,A}(z_{0,A}) \) with the same radius \( R \) in \( \mathbb{R}^{2n,A} \) and centered at the projection \( z_{0,A} \) of \( z_0 \). The next step involves replacing the total Hamiltonian \( \hat{H} \) in (4) with a local approximation \( \hat{H}_0 \) for each \( z_0 \). This local Hamiltonian is obtained as follows: let \( z_t \) be the solution of the Hamilton equations for \( \hat{H} \) passing through \( z_0 \) at time \( t = 0 \). \( \hat{H}_0 \) is then advantages, one of them being that Weyl quantization is symplectically covariant under conjugation with metaplectic operators.
obtained by truncating the Taylor series of $H(z)$ at $z = z_t$ and retaining only terms of order $\leq 2$:

$$H_0(z, t) = H(z_t, t) + \nabla_z H(z_t, t)(z - z_t) + \frac{1}{2} H''(z_t, t)(z - z_t)^2.$$ 

If we take $z_0$ as the initial condition for the Hamilton equations for $H_0$, the exact solution is $z_t$. If we choose an initial point close to $z_0$ we will get a (hopefully good) approximation to the exact solution (intuitively the smaller the radius $R$ the better this approximation will be). This procedure is what Littlejohn [44] calls the “nearby orbit approximation”; when applied to the semiclassical case it is a generalization of Heller’s thawed Gaussian approximation [33, 37]; also see Hepp [38]. Now, the local Hamiltonian $H_0$ is a quadratic polynomial in the phase space variables, and the corresponding Hamilton equations are thus linear so that the local Hamiltonian flow $\Phi_t$ they generate can be expressed using only phase space translations and linear symplectic transformations. Taking for simplicity $z_0 = 0$, after time $t$ this flow $\Phi_t$ will thus have deformed the initial ball $B_R^{2n}(0)$ into a phase space ellipsoid

$$\Omega_t = \{z_t\} + S_t B_R^{2n}(0)$$

where $S_t$ is a symplectic matrix in $\mathbb{R}^{2n}$. Now comes the crucial point: very recent results [14] in symplectic geometry show that the shadow $\Omega_{A,t}$ of $\Omega_t$ on $\mathbb{R}^{2n_A}$ is an ellipsoid containing a symplectic ball centered at $z_{A,t}$:

$$\Omega_{A,t} \supset z_{A,t} + S_{A,t} B_R^{2n_A}(0)$$

where $S_{A,t}$ is a symplectic matrix in the smaller phase space $\mathbb{R}^{2n_A}$ and $z_{A,t}$ the projection of $z_t$. This striking (and highly non-trivial) result follows from a generalization [14] (in the linear case) of Gromov’s [29] famous “principle of the symplectic camel”. We sketch the proof of this result in Theorem 3. The quantum analogue of a symplectic ball is what we have called a “quantum blob” in earlier work [20], and the Wigner formalism shows that quantum blobs are in one-to-one correspondence with pure Gaussian states (sometimes called generalized squeezed coherent states). This allows us to propagate these Gaussians semiclassically using a Weyl quantization

$$\hat{H}_0 = H(z_t, t) + \nabla_z H(z_t, t)(\hat{z} - z_t) + \frac{1}{2} H''(z_t, t)(\hat{z} - z_t)^2$$

of the local Hamiltonian. The main result is then that a pure Gaussian state in the subsystem $A$ will evolve into a mixed (Gaussian) which will be described explicitly in Theorem 6 using the semiclassical propagator which can be expressed using only displacement and metaplectic operators.
Notation and terminology. The phase space variable will be written \( z = (z_A, z_B) \) with \( z_A = (x_A, p_A) \) and \( z_B = (x_B, p_B) \). We will also use the notation \( z = z_A \oplus z_B \) and
\[
J = J_A \oplus J_B = \begin{pmatrix} J_A & 0 \\ 0 & J_B \end{pmatrix}
\]
where \( J_A \) (resp. \( J_B \)) is the standard symplectic matrix on \( \mathbb{R}^{2n_A} \) (resp. \( \mathbb{R}^{2n_B} \)). They correspond to the symplectic structures \( \sigma(z, z') = J z \cdot z' \), \( \sigma_A(z_A, z'_A) = J_A z_A \cdot z'_A \), and \( \sigma_B(z_B, z'_B) = J_B z_B \cdot z'_B \), respectively. The scalar product of two vectors \( u, v \in \mathbb{R}^m \) is written \( u \cdot v \) or \( uv \); if \( A \) is a symmetric \( m \times m \) matrix we use the shorthand notation \( Au \cdot u = Au^2 \). The symplectic group of the symplectic space \( (\mathbb{R}^{2n}, \sigma) \) is denoted by \( \text{Sp}(n) \); similarly the symplectic groups of \( (\mathbb{R}^{2n_A}, \sigma_A) \) and \( (\mathbb{R}^{2n_B}, \sigma_B) \) are \( \text{Sp}(n_A) \) and \( \text{Sp}(n_B) \), respectively.

We denote by \( B_{2n}^R(z_0) \) the open ball in \( \mathbb{R}^{2n} \) with radius \( R \) and center \( z_0 \):
\[
B_{2n}^R(z_0) = \{ z \in \mathbb{R}^{2n} : |z - z_0| < R \}.
\]
When \( z_0 = 0 \) we write \( B_{2n}^R(0) = B_{2n}^R \) and
\[
B_{2n}^R(z_0) = \{ z_0 \} + B_{2n}^R.
\]
The volume of \( B_{2n}^R(z_0) \) is
\[
\text{Vol}(B_{2n}^R(z_0)) = \left( \frac{\pi R^2}{n!} \right)^n.
\]
We call the image \( S(B_{2n}^R(z_0)) \) of \( B_{2n}^R(z_0) \) by a linear canonical transformation \( S \in \text{Sp}(n) \) a symplectic ball with center \( S z_0 \) and radius \( R \). By Liouville’s theorem \( S(B_{2n}^R(z_0)) \) and \( B_{2n}^R(z_0) \) have the same volume.

1 The Extended Symplectic Camel Principle

1.1 Statement and discussion

In 1985 the mathematician M. Gromov \cite{Gromov} proved the following remarkable and highly non-trivial result, known as the “symplectic non-squeezing theorem”:

**Theorem 1 (Gromov)** No canonical transformation \( \Phi \) of \( \mathbb{R}^{2n} \) (linear, or not) can squeeze a phase space ball \( B_{2n}^R(z_0) \) through a circular hole in a plane of conjugate coordinates \( x_j, p_j \) with radius smaller than \( R \).
Gromov’s theorem, whose proof is highly non-trivial, is often restated as the “principle of the symplectic camel (PSC)” [18, 28]:

**Theorem 2 (Symplectic camel)** Let \( \Phi \) be a canonical transformation of \( \mathbb{R}^{2n} \) and \( \Pi_j \) the orthogonal projection \( \mathbb{R}^{2n} \to \mathbb{R}_{x_j,p_j}^2 \) on any plane of conjugate variables \( x_j, p_j \). We have

\[
\text{Area } \Pi_j(\Phi(B_{2n}^n(z_0))) \geq \pi R^2.
\]

(9)

These results at first sight seem to contradict the common conception of Liouville’s theorem on volume conservation; they are in fact refinements of it. The PSC has in fact the following dynamical interpretation: assume that we are moving the ball \( B_{2n}^n(z_0) \) through phase space using some Hamiltonian flow \( \Phi_t \), which is a one-parameter family of canonical transformations. In view of Liouville’s theorem the deformed ball \( \Phi_t(B_{2n}^n(z_0)) \) will have the same volume as \( B_{2n}^n(z_0) \); the principle of the symplectic camel says that in addition its “shadow” (orthogonal projection) on any \( x_j, p_j \) plane will never decrease below its initial value \( \pi R^2 \). The result ceases to be true if we move the ball using non-Hamiltonian volume-preserving flows: it is the symplectic character of Hamiltonian flows which plays an essential role here. It does not require very much imagination to realize that the PSC is reminiscent of the quantum uncertainty principle. In fact, we have shown in [17, 18, 28] that Heisenberg’s uncertainty principle in its strong form (the Robertson–Schrödinger inequalities) can be concisely reformulated using the PSC, and that this reformulation also extends to the case of classical uncertainties [19]. We mention that Kalogeropoulos [11] has been able to use the principle of the symplectic camel to study a non-standard characterization of thermodynamical entropy (also see the related paper [40]).

The planes of conjugate coordinates \( x_j, p_j \) just considered are particularly simple examples of phase subspaces of \( \mathbb{R}^{2n} \) and correspond to the case \( n_A = 1 \) in the notation of the Introduction. A natural question which arises is whether the PSC can be extended to symplectic subspaces of higher dimension, \( i.e. \) to arbitrary phase sub-spaces \( \mathbb{R}^{2n_A} \). For general nonlinear canonical transformations the situation is not yet very well understood (this will be discussed in Section 3). However, in a recent work [14] we have proved, in collaboration with N. Dias and J. Prata, the following refinement of the PSC for linear canonical transformations:

**Theorem 3 (Extended symplectic camel)** Let \( \Pi_A \) be the orthogonal projection \( \mathbb{R}^{2n_A} \times \mathbb{R}^{2n_B} \to \mathbb{R}^{2n_A} \). There exists \( S_A \in \text{Sp}(n_A) \) such that for
every $R > 0$ the projected ellipsoid $\Pi_A(S(B^{2n}_R))$ contains the symplectic ball $S_A(B^{2n}_R)$:

$$\Pi_A(S(B^{2n}_R)) \supset S_A(B^{2n}_R).$$

(10)

More generally,

$$\Pi_A(S(B^{2n}_R(z_0))) \supset \{ \Pi_A(Sz_0) \} + S_A(B^{2n}_R).$$

(11)

We have equality in (10), (11) if and only if $S = S_A \oplus S_B$ for some $S_B \in \text{Sp}(n_B)$.

Note that (11) immediately follows from (10) so that it is sufficient to focus our attention on the proof of the inclusion (10). The idea of the proof goes as follows (see [14] for details): the ball $\Omega = S(B^{2n}_R)$ is determined by the inequality $Pz^2 \leq R^2$ where $P = (SS^T)^{-1}$. Writing $P$ in block matrix form

$$P = \begin{pmatrix} P_{AA} & P_{AB} \\ P_{BA} & P_{BB} \end{pmatrix}$$

(12)

the blocks $P_{AA}, P_{AB}, P_{BA}, P_{BB}$ having dimensions $2n_A \times 2n_A, 2n_A \times 2n_B, 2n_B \times 2n_A, 2n_B \times 2n_B$, respectively, the projection $\Omega_A = \Pi_A(S(B^{2n}_R))$ on $\mathbb{R}^{2n_A}$ is then the ellipsoid

$$\Omega_A = \{ z_A : (P/P_{BB})z_A^2 \leq R^2 \}$$

(13)

where the $2n_A \times 2n_A$ symmetric and positive definite matrix $P/P_{BB}$ is the Schur complement of $P_{BB}$ in $P$, that is

$$P/P_{BB} = P_{AA} - P_{AB}P_{BB}^{-1}P_{BA}.$$ 

(14)

It follows that $\Omega_A$ is a non-degenerate ellipsoid in $\mathbb{R}^{2n_A}$. In view of Williamson’s diagonalization theorem [17] there exists a symplectic matrix $S_A \in \text{Sp}(n_A)$ diagonalizing $P/P_{BB}$, that is

$$P/P_{BB} = (S_A^{-1})^T D_A S_A^{-1}$$

(15)

where $D_A$ has the form

$$D_A = \begin{pmatrix} \Lambda_A & 0 \\ 0 & \Lambda_A \end{pmatrix}$$

(16)

with $\Lambda_A = \text{diag}(\lambda_1, \ldots, \lambda_{n_A})$, the positive numbers $\lambda_j$ being the symplectic eigenvalues of $P/P_{BB}$ (i.e. the positive numbers $\lambda_j$ such that $\pm i \lambda_j$ is an
eigenvalue of $J_A(P/P_{BB})$. The symplectic matrix $S_A$ in (15) is the one appearing in (10), (11), and one proves that $D_A \leq I$, that is
\begin{equation}
\lambda_j \leq 1 \text{ for } j = 1, \ldots, n_A .
\end{equation}

The proof of the inclusion (10) now follows: in view of (15) the inequality (13) is equivalent to
\begin{equation}
(S_A^{-1})^T D_A S_A^{-1} z_A^2 \leq R^2 ;
\end{equation}

since $D_A \leq I$ it implies that the projection $\Omega_A$ must contain the ball $\Omega_A = S_A(B_{R_n}^{2n,A})$.

Note that since symplectic mappings are volume-preserving we have
\begin{equation}
\text{Vol } \Pi_A(S(B_{R_n}^{2n})) \geq \text{Vol } B_{R_n}^{2n,A} .
\end{equation}

This inequality qualifies Theorem 3 as an extension of the principle of the symplectic camel: since $S_A$ is volume preserving in $\mathbb{R}^{2n,A}$ it reduces to Theorem 2 when $n_A = 1$ in the linear case. The inequality (18) was in fact proved directly by Abbondandolo and Matveyev [2] some time ago, using methods from differential geometry. We mention that Abbondandolo and Benedetti [1] have very recently improved the inequality (18) by showing that a similar inequality still holds for canonical transformations close to linear ones. It is an open question whether Theorem 3 can be improved to encompass such transformations (see the discussion in Section 3).

1.2 The nearby orbit method

Consider the generalized time-dependent harmonic oscillator with Hamiltonian
\begin{equation}
H(z, t) = \frac{1}{2} M(t) z^2
\end{equation}

where $M = M(t)$ is a real symmetric $2n \times 2n$ matrix depending continuously on time $t$. The associated Hamilton equations are linear and hence a solution $z(t)$ of the associated Hamilton equations satisfies $z(t) = S_t z(0)$ with $S_t \in \text{Sp}(n)$. As an immediate application of the extended principle of the symplectic camel (formula (11) in Theorem 3) there exists a one-parameter family of matrices $S_{A,t} \in \text{Sp}(n_A)$ such that
\begin{equation}
\Pi_A(S_t(B_{R_n}^{2n}(z_0))) \supset \{ \Pi_A(S_t z_0) \} + S_{A,t}(B_{R_n}^{2n,A}) .
\end{equation}

Let now $H = H(z, t)$ be an arbitrary (possibly time-dependent) Hamiltonian function on $\mathbb{R}^{2n}$. We assume $H$ to be at least twice continuously
differentiable in the position and momentum variables and once continuously differentiable with respect to time $t$. Fixing a reference point $z_0$ in phase space we denote by $z_t$ the solution to Hamilton’s equation for $H$ with initial datum $z_0$ at time $t = 0$. We will call the phase space curve $t \mapsto z_t$ the **reference orbit**. We define the flow mapping $\Phi_t : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ by $z(t) = \Phi_t(z(0))$ where $z(t)$ is the solution of Hamilton’s equations for the initial Hamiltonian $H$. The mappings $\Phi_t$ are canonical transformations \[3, 17\]. This follows from the fact that the Jacobian matrix

$$S_t(z_0) = \partial(x_t, p_t)/\partial(x_0, p_0)$$

(21)
is symplectic, that is $S_t(z_0) \in \text{Sp}(n)$ for all times $t$. This property easily follows from the fact that $S_t$ satisfies the “variational equation” (see \[17\], §2.3.2)

$$\frac{d}{dt}S_t(z_0) = JH'''(z_t, t)S_t(z_0)$$

(22)
where

$$H''' = (\partial^2 H/\partial z_\alpha \partial z_\beta)_{1 \leq \alpha, \beta \leq 2n}$$

(23)
is the Hessian matrix of $H$, i.e. the matrix of second derivatives of $H$ in the phase space variables $z_\alpha = x_\alpha$ for $\alpha = 1, \ldots, n$ and $z_\alpha = p_\alpha$ for $\alpha = n + 1, \ldots, 2n$.

This leads us to consider the truncated Taylor expansion

$$H_0(z, t) = H(z_t, t) + \nabla_z H(z_t, t)(z - z_t) + \frac{1}{2}H'''(z_t, t)(z - z_t)^2$$

(24)
of the original Hamiltonian $H$ around the point $z_t$. This new Hamiltonian $H_0$ is time-dependent, even if $H$ is not. In the particular case where $H$ has the simple physical form

$$H(x, p, t) = \frac{1}{2}m^{-1}p^2 + V(x, t)$$

(25)
($m$ the mass matrix) the approximate Hamiltonian \[24\] takes the familiar form \[4, 44\]

$$H_0(x, p, t) = \frac{1}{2}m^{-1}(p - p_t)^2 + V_{LHA}(x, t)$$

(26)

\[While Hamilton’s equations can usually not be solved exactly, there are efficient numerical symplectic algorithms allowing to determine the reference orbit $z_t$ with very good precision. See for instance \[8, 41, 54, 46\] and the references therein.\]
where \( V_{\text{LHA}}(x, t) \) is the time-dependent local harmonic approximation of the potential \( V(x) \):

\[
V_{\text{LHA}}(x, t) = V(x_t) + \nabla_x V(x_t)(x - x_t) + \frac{1}{2}V''(x_t)(x - x_t)^2.
\] (27)

The solutions to the Hamilton equations for \( H \) and \( H_0 \) coincide when the initial value of \( z(t) \) is chosen equal to the reference point \( z_0 \) for both systems. In fact, the Hamilton equations for \( H_0 \) are

\[
\dot{u}_t = J \nabla z H(z_t, t)(u_t - z_t) + J H''(z_t, t)(u_t - z_t)
\] (28)

and replacing \( u_t \) with \( z_t \) yields \( \dot{z}_t = J \nabla z H(z_t, t) \). Now, the solution of the Hamilton equations (28) with initial datum \( u_0 \) is easily calculated and one finds that

\[
u_t = z_t + S_t(z_0)(u_0 - z_0).
\] (29)

Setting \( u_t = U_t(z_0)(u_0) \) and introducing the phase space translations \( T(u) : z \mapsto z + u \) this formula can be rewritten as

\[
U_t(z_0) = T(z_t)S_t(z_0)T(-z_0)
\] (30)

so that \( U_t(z_0) \) can be viewed as a classical propagator \[44\]. Recalling that we have set \( z(t) = \Phi_t(z(0)) \) the discussion above shows that \( \Phi_t(z) = U_t(z_0)(z) \) when \( z = z_0 \), which suggests to approximate the flow \( \Phi_t \) by the affine mappings \( U_t(z_0) \) for points close to \( z_0 \): this is the idea of the “nearby orbit approximation” with respect to reference orbit \( t \mapsto z_t \). The validity of this approximation can be tested using the standard theory of systems of differential equations using the equality (29); the Lyapunov exponents are crucial for the study of the accuracy of the solutions. In the absence of chaotic behavior it is actually quite good for short times (Miller \[47\]) which makes it work well for low and or medium resolution electronic spectra. The following straightforward consequence of the extended symplectic camel principle is new; it describes the approximate motion of the projection on \( \mathbb{R}^{2n_A} \) of \( \Phi_t(B_{\mathbb{R}}^{2n}(z_0)) \):

**Theorem 4** Let \( U_t(z_0) \) be the flow determined by \( H \) in the nearby orbit approximation with reference orbit \( t \mapsto z_t \) starting from \( z_0 \). The orthogonal projection

\[
\Omega_{A,t}(z_0) = \Pi_A(U_t(z_0)(B_{\mathbb{R}}^{2n}(z_0)))
\]

contains a symplectic ball centered at \( z_{A,t} = \Pi_A(z_t) \):

\[
\Omega_{A,t}(z_0) \supset \{ z_{A,t} \} + S_{A,t}(z_0)(B_{\mathbb{R}}^{2n_A})
\] (31)

where \( S_{A,t}(z_0) \in \text{Sp}(n_A) \).
Proof. Since $T(-z_0)B^{2n}_R(z_0) = B^{2n}_R$ formula (30) yields

$$U_t(z_0)(B^{2n}_R(z_0)) = T(z_t)S_t(z_0)(B^{2n}(0, R))$$

$$= \{z_t\} + S_t(z_0)(B^{2n}_R) .$$

Formula (31) now follows from the inclusion (20) taking into account the linearity of the projection $\Pi_A$. ■

Formula (31) implies the following important property of the subsystem $A$: while the motion of the “shadow” of the initial ball $B^{2n}_R(z_0)$ on $\mathbb{R}^{2n,A}$ cannot be Hamiltonian (it is not volume preserving), it however contains a symplectic ball whose evolution is governed by a Hamiltonian flow, namely that determined by

$$H_A(z_A, t) = -\frac{1}{2}J_A\dot{S}_{A,t}(z_0)S_{A,t}(z_0)^{-1}(z_A - z_{A,t})^2 + J_A z_A \cdot \dot{z}_{A,t}$$

where $\dot{S}_{A,t}(z_0) = \frac{d}{dt}S_{A,t}(z_0)$. In fact,

$$J_A \nabla_{z_A} H_A(z_A, t, t) = \dot{S}_{A,t}(z_0)S_{A,t}(z_0)^{-1}(z_A - z_{A,t}) + \dot{z}_{A,t}$$

and hence the solution $z_A(t)$ of the Hamilton equations for $H_A$ satisfies the linear differential equation

$$\frac{d}{dt}(z_A(t) - z_{A,t}) = \dot{S}_{A,t}(z_0)S_{A,t}(z_0)^{-1}(z_A(t) - z_{A,t}) .$$

The solution of this equation is $z_A(t) = z_{A,t} + S_{A,t}(z_0)$ and hence our claim³.

1.3 Entropy increase in subsystems

In the nearby orbit approximation the orthogonal projection $\Omega_{A,t}(z_0)$ of $U_t(z_0)(B^{2n}_R(z_0))$ is the ellipsoid defined by the inequality

$$(P_t(z_0)/P_{BB,t}(z_0))(z_A - z_{A,t})^2 \leq R^2$$

(32)

where we have written the symplectic matrix

$$P_t(z_0) = (S_{A,t}(z_0)S_{A,t}(z_0)^T)^{-1}$$

³On a more fundamental level this result is a consequence of the fact that any smooth family $S_t$ of symplectic matrices such that $S_0 = I$ is the flow determined by some quadratic Hamiltonian [21].
in block matrix form
\[
P_t(z_0) = \begin{pmatrix} P_{AA,t}(z_0) & P_{AB,t}(z_0) \\ P_{BA,t}(z_0) & P_{BB,t}(z_0) \end{pmatrix}.
\] (33)

The volume of \( \Omega_{A,t}(z_0) \) is thus
\[
\text{Vol } \Omega_{A,t}(z_0) = \det(P_t(z_0)/P_{BB,t}(z_0)) \text{Vol } B_{R}^{2n_{A}}.
\]

Recalling that the Schur complement satisfies the relation [58]:
\[
\det P_t(z_0) = \det(P_t(z_0)/P_{BB,t}(z_0)) \det P_{BB,t}(z_0);
\] (34)
in the present case \( P_t(z_0) \) is symplectic so that \( \det P_t(z_0) = 1 \), and we thus have
\[
\det(P_t(z_0)/P_{BB,t}(z_0)) \det P_{BB,t}(z_0) = 1
\] (35)
and hence
\[
\text{Vol } \Omega_{A,t}(z_0) = \frac{1}{\det P_{BB,t}(z_0)} \text{Vol } B_{R}^{2n_{A}}.
\] (36)

The entropy increase\(^4\) is thus
\[
\Delta S = -k_B \ln(\det P_{BB,t}(z_0))
\] (37)
where ln is the natural logarithm. This increase is due only to the subsystem \( B \). If \( A \) and \( B \) are uncoupled, then the cross-term \( P_{AB,t}(z_0) = P_{BA,t}(z_0)^T = 0 \) so that both \( P_{AA,t}(z_0) \) and \( P_{BB,t}(z_0) \) are both symplectic and we have
\[
P_t(z_0) = P_{AA,t}(z_0) \oplus P_{BB,t}(z_0)
\]
so that \( \text{Vol } \Omega_{A,t} = \text{Vol } B_{R}^{2n_{A}} \) remains constant. This phenomenon shows the hardly surprising fact that the Boltzmann entropy of the subsystem \( A \) can take arbitrarily large values as the subsystem \( A \) occupies an increasing volume of phase space due to interaction with the subsystem \( B \).

There is another way to express this result using the symplectic eigenvalues \( \lambda_{j,t}(z_0) \) of \( P_{BB,t}(z_0) \). In view of formula (15) we have
\[
P_t(z_0)/P_{BB,t}(z_0) = (S_{A,t}(z_0)^{-1})^T D_{A,t}(z_0) S_{A,t}(z_0)^{-1}
\]
with
\[
D_{A,t}(z_0) = \begin{pmatrix} \Lambda_{A,t}(z_0) & 0 \\ 0 & \Lambda_{A,t}(z_0) \end{pmatrix}
\] (38)
\[
\Lambda_{A,t}(z_0) = \text{diag}(\lambda_{1,t}(z_0), ..., \lambda_{n_{A,t}}(z_0)).
\] (39)

\(^4\)That the entropy increases already follows from the estimates in Abbondandolo and Matveyev [2] on the volume of the projection of a symplectic ball.
It follows that the volume of $\Omega_{A,t}$ is
\[
\text{Vol} \Omega_{A,t}(z_0) = \det(D_{A,t}(z_0))^{-1/2} \text{Vol} B_R^{2n_A} \frac{1}{\lambda_{1,t}(z_0) \cdots \lambda_{n_{A,t}}(z_0)} \text{Vol} B_R^{2n_A}.
\]
This volume can become arbitrarily large regardless of the dimension $n_B$ of the system $B$. For this it suffices that at least one of the symplectic eigenvalues $\lambda_{j,t}(z_0)$ is sufficiently small. The entropy increase can thus be expressed as
\[
\Delta S = -k_B \sum_{j=1}^{n_A} \ln \lambda_{j,t}(z_0).
\]

One should however be aware of the fact that symplectic topology teaches us, via Gromov’s non-squeezing theorem, that in Hamiltonian dynamics the true measure of spreading is not volume, but symplectic capacity \[18\] \[28\]. Let us shortly discuss our results from this new point of view. By definition, the symplectic capacity $\text{Cap} \Omega$ (or Gromov width) of a phase space ellipsoid $\Omega$ (in any dimension) is the number $\pi r_{\text{max}}^2$ where $r_{\text{max}}$ is the radius of the largest phase space ball that can be embedded inside that ellipsoid using canonical transformations (linear, or not). The symplectic capacity of the ellipsoid

$$\Omega = \{ z : Mz^2 \leq R^2 \}$$

($M = M^T$ positive definite) is explicitly given by the formula
\[
\text{Cap} \Omega = \frac{\pi R^2}{\lambda_{\text{max}}}
\]
where $\lambda_{\text{max}}$ is the largest symplectic eigenvalue of the matrix $M$. Notice that $\text{Cap} \Omega$ does not depend on the dimension of the ambient phase space, it is thus an extrinsic quantity, as opposed to volume. For instance $\text{Cap} B_R^{2n} = \pi R^2$ but also $\text{Cap} Z_R^{2n} = \pi R^2$ where $Z_R^{2n}$ is the centered cylinder with radius $R$ based on a plane of conjugate coordinates (the latter follows from Gromov’s theorem, and is actually equivalent to it). The symplectic capacity of an unbounded set can thus be finite, showing that the notion of symplectic capacity is very different from that of volume (except in the case $n = 1$ where it is essentially an area: see our discussion in \[18\] \[28\]). To illustrate this, let us calculate $\text{Cap} \Omega_{A,t}$. In view of formula (41) and taking into account the translational invariance \[17\] of the symplectic capacities formula (41) yields
\[
\text{Cap} \Omega_{A,t} = \frac{\pi R^2}{\lambda_{\text{max},t}(z_0)}
\]
where
\[
\lambda_{\text{max},t}(z_0) = \max_j \{ \lambda_{j,t}(z_0), 1 \leq j \leq n_A \}.
\]
2 The Semiclassical Case

We denote by \( \hat{T}(z_0) = e^{-i\sigma(z,z_0)/\hbar} \) the Heisenberg displacement operator on \( L^2(\mathbb{R}^n) \). It is explicitly given by the formula \[ \hat{T}(z_0)\psi(x) = e^{i(p_0x - p_0x_0/2)/\hbar} \psi(x - x_0). \] (42)

We recall [17, 21, 44] that the symplectic group \( \text{Sp}(n) \) has a two-fold covering whose elements are unitary operators acting on \( L^2(\mathbb{R}^n) \). This group is called the metaplectic group \( \text{Mp}(n) \). To every \( S \in \text{Sp}(n) \) corresponds exactly two metaplectic operators \( \pm \hat{S} \in \text{Mp}(n) \) and we have the following intertwining property:

\[ \hat{T}(z) \hat{S} = \hat{S} \hat{T}(S^{-1}z) \] (43)

which is the analogue at the operator level of the obvious relation

\[ T(z)S = ST(S^{-1}z). \]

2.1 A generalization of the thawed Gaussian approximation

We now consider the quantized version \( \hat{H} \) of the Hamiltonian \( H \). We will approximate \( \hat{H} \) by quantizing the nearby-orbit Hamiltonian (24), which yields the operator

\[ \hat{H}_0 = H(z_t, t) + \nabla_z H(z_t, t)(\tilde{z} - z_t) + \frac{1}{2} H''(z_t, t)(\tilde{z} - z_t)^2 \] (44)

where \( \tilde{z} = (\tilde{x}, \tilde{p}) \) with \( \tilde{x} = (\tilde{x}_1, ..., \tilde{x}_n) \) (\( \tilde{x}_j \) multiplication by \( x_j \)) and \( \tilde{p} = -i\hbar \nabla_x \). When \( H \) has the simple physical form (25) this reduces to the simple operator

\[ \hat{H}_0 = \frac{1}{2} M^{-1}(\tilde{p} - p_0)^2 + V_{\text{LHA}}(\tilde{x}, t) \] (45)

where \( V_{\text{LHA}}(x, t) \) is given by (27). Let now \( \psi_0 \) be a wavepacket (for instance, but not necessarily, a Gaussian). Assuming that \( \psi \) is well-localized around \( x_0 \) and its Fourier transform around \( p_0 \) one postulates that a good approximation to the solution of the full Schrödinger equation

\[ i\hbar \partial_t \psi = \hat{H} \psi, \quad \psi(\cdot, 0) = \psi_0 \]

is obtained by replacing \( \hat{H} \) with its approximation \( \hat{H}_0 \). It is not difficult (Littlejohn [44], §7) to see that the approximate solution is then given by the quantum analogue of the equivalent formulas (29) and (30):

\[ \psi(x, t) = e^{\frac{i}{\hbar}\gamma(t)} \hat{T}(z_t) \hat{S}_t(z_0) \hat{T}(-z_0) \psi_0(x) \] (46)

\footnote{This supplementary condition is often forgotten in practice; it is equivalent to saying that the Wigner transform of \( \psi \) is concentrated near \( z_0 = (x_0, p_0) \).}
where \( \gamma(t) \) is a phase correction, and \( \hat{S}_t(z_0) \) the metaplectic lift of the path \( S_t(z_0) \). We will call the mapping

\[
\hat{U}_t(z_0) = e^{i\gamma(t)} \hat{T}(z_t) \hat{S}_t(z_0) \hat{T}(-z_0)
\]

(47)

the semiclassical propagator relative to the reference orbit \( z_t \). This formula is interpreted as follows \([17, 21]\): let \( S_t \) be the phase space flow determined by a quadratic Hamiltonian of the type (19), that is \( H(z, t) = \frac{1}{2} M(t) z^2 \). According to general principles from the theory of covering spaces, this one-parameter family of symplectic matrices can be lifted in a unique way to a one-parameter family of operators \( \hat{S}_t \) in \( \text{Mp}(n) \) such that \( \hat{S}_0 = I_d \). The lifting is constructed as follows: since \( \text{Mp}(n) \) is a double covering of \( \text{Sp}(n) \) to each symplectic matrix \( S_t \) corresponds two metaplectic operators; for each time \( t \) one then chooses the operator leading to a continuous path \( \hat{S}_t \) passing through the identity of \( \text{Mp}(n) \) at time \( t = 0 \); for details of the construction, see \([17]\), especially §7.2.2. This being done, one then shows (ibid.) that for any square integrable initial wavepacket \( \psi_0 \) the function \( \psi(x, t) = \hat{S}_t \psi_0(x) \) is a solution of the Schrödinger equation with Hamiltonian operator \( \hat{H} = \frac{1}{2} M(t) \hat{x}^2 \). Formula (47) follows applying that lifting principle to the classical flow (30) noting that following a similar argument the one-parameter family \( T(z_t) \) (which is the flow of the displacement Hamiltonian \( H_t(z) = px_t - p_t x \)) lifts to the one-parameter family \( \hat{T}(z_t) \) (which is the propagator for the Hamiltonian operator \( \hat{H}_t = \hat{p}x_t - p_t \hat{x} \)).

As already noted by Littlejohn \([44]\) this construction is essentially that of Heller and his collaborators \([33, 34, 35, 36, 39]\) (also see Heller’s recent monograph \([37]\)) known as the “thawed Gaussian approximation” when the Hamiltonian is of the physical type “kinetic energy plus potential”. The difference is that Heller built the time evolution into the parameters of a Gaussian wave packet, while we have placed it into the operator, which has the advantage that the initial wavefunction need not be Gaussian, and allows much more general Hamiltonians. Such approximations (and their generalizations to higher orders) have been extensively studied in physics and mathematics; a non-exhaustive list of related papers is \([6, 10, 13, 30, 31, 32, 33, 35, 51, 52]\). They have applications to on-the-fly \( ab \ initio \) semiclassical calculations of molecular spectra \([5, 55, 56]\); also see the recent paper \([50]\) by Patoz et al. For a very recent and up-to-date survey with applications to computable algorithms see Lasser and Lubich \([42]\); their paper in addition contains rigorous error estimates.

We mention that in a recent work \([5]\) Begušić \textit{et al.} have considered a simplified variant of Heller’s approximation obtained by “freezing” the
Hessian $V''(x_t)$ of the potential in (27) at the initial position $x_0$; the authors argue that this decreases the computational complexity, but at the cost of a loss of accuracy. In our generalized context this would amount to replacing the approximate Hamiltonian $H$ in (24) with

$$K_0(z, t) = H(z_t, t) + \nabla_z H(z_t, t)(z - z_t) + \frac{1}{2} H''(z_0, t)(z - z_t)^2 \quad (48)$$

and the use of its quantized version $\hat{K}_0$ to propagate wavepackets. Our arguments still apply mutatis mutandis if one uses $K_0$ instead of $H_0$ since $K_0$ also is quadratic in the position and momentum variables and thus allows the use of the metaplectic machinery.

### 2.2 Gaussian mixed states and the Wigner ellipsoid

It is well-known that there is a one-to-one correspondence between minimum uncertainty phase space ellipsoids and Gaussian states; perhaps one of the first systematic studies of this correspondence is Littlejohn’s seminal paper [44]. We have exploited this property in [17, 18, 19, 28] using the properties of the Wigner transform. Working in canonical global coordinates $z = (x, p)$ the Wigner transform of $\psi \in L^2(\mathbb{R}^n)$ is, by definition,

$$W\psi(x, p) = \left(\frac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar} p \cdot y} \psi(x + \frac{1}{2} y) \psi^*(x - \frac{1}{2} y) dy . \quad (49)$$

It satisfies the following transformation formulas [17, 26, 44]

$$W(\hat{S}\psi)(z) = W(\psi(S^{-1}z)) \quad (50)$$
$$W(\hat{T}(z_0)\psi)(z) = W(\psi(z - z_0)) . \quad (51)$$

Here is a simple but fundamental example: let $\psi = \phi_0$ be the standard centered coherent state:

$$\phi_0(x) = (\pi\hbar)^{-n/4} e^{-|x|^2/2\hbar} ; \quad (52)$$

its Wigner transform is the Gaussian

$$W\phi_0(z) = (\pi\hbar)^{-n} e^{-|z|^2/\hbar} . \quad (53)$$

---

6Littlejohn [44] calls it the “fiducial coherent state”.

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More generally, the standard coherent state centered at \( z_0 = (x_0, p_0) \) is
\[
\phi_{z_0}(x) = e^{-ip_0 x_0/2\hbar} e^{ip_0 x/\hbar} \phi_0(x - x_0)
\]
and its Wigner transform is, using (51),
\[
W\phi_{z_0}(z) = (\pi \hbar)^{-n} e^{-|z - z_0|^2/\hbar}.
\]

More generally consider (normalized) generalized Gaussian states \(|\psi_{X,Y}\rangle\) with
\[
\psi_{X,Y}(x) = \left(\frac{1}{\pi \hbar}\right)^{n/4} (\det X)^{1/4} e^{-\frac{1}{2\hbar} M x^2}
\]
where \( M = X + iY \), \( X \) and \( Y \) real symmetric, \( X \) positive definite. These states generalize the “squeezed states” familiar from quantum optics, the “squeezing parameters” being the eigenvalues of \( X \). The Wigner transform of \( \psi_{X,Y} \) is explicitly given by [15, 17, 44]
\[
W\psi_{X,Y}(z) = \left(\frac{1}{\pi \hbar}\right)^n e^{-\frac{1}{2\hbar} G z^2}
\]
where \( G \) is a symmetric symplectic matrix:
\[
G = R^T R, \quad R = \begin{pmatrix} X^{1/2} & 0 \\ -X^{-1/2} Y & X^{-1/2} \end{pmatrix}.
\]

The “covariance (or Wigner) ellipsoid” [44]
\[
\Omega_\Sigma = \{ z : G z^2 \leq \hbar \}
\]
of \( \psi_{X,Y} \) is the symplectic ball:
\[
\Omega_\Sigma = S(B_{2n}^{2n})^\circ, \quad S = R^{-1} \in \text{Sp}(n).
\]

Conversely, if an ellipsoid \( \Omega \) is a symplectic ball \( SB_{2n}^{2n} \), then the function \( \rho(z) = (\pi \hbar)^{-n} e^{-G z^2/\hbar} \) with \( G = (S^{-1})^T S^{-1} \) is the Wigner transform of a Gaussian [54] up to an unessential prefactor with modulus one.

Let us consider more general phase space Gaussians
\[
\rho(z) = (\pi \hbar)^{-n} (\det M)^{1/2} e^{-\frac{1}{2\hbar} M z^2}.
\]

Defining the covariance matrix of \( \rho \) by
\[
\Sigma = \frac{\hbar}{2} M^{-1}
\]
we can rewrite (57) in the perhaps more familiar form
\[ \rho(z) = \frac{1}{(2\pi)^n \sqrt{\det \Sigma}} e^{-\frac{1}{2} \Sigma^{-1} z^2}. \] (59)

An essential result in harmonic analysis [4, 16, 17, 23, 24, 48] is now that \( \rho(z) \) is the Wigner distribution of a mixed quantum state if and only if the “quantum condition”
\[ \Sigma + \frac{i\hbar}{2} J \geq 0 \iff M^{-1} + i J \geq 0 \] (60)
holds (“\( \geq 0 \)” means “is positive semidefinite”; note that the eigenvalues of \( \Sigma + \frac{i\hbar}{2} J \) are real since \( (iJ)^* = -iJ^T = iJ \)). When (60) holds, the purity of the Gaussian state \( \hat{\rho} \) with Wigner distribution (59) is ([27] and [17], §9.3, p.301)
\[ \mu(\hat{\rho}) = \left( \frac{\hbar}{2} \right)^n (\det \Sigma)^{-1/2} = \sqrt{\det M}; \] (61)

it follows that \( \hat{\rho} \) is a pure state \( \psi_M \) if and only if \( \det M = 1 \). Defining the Wigner ellipsoid [44] of \( \hat{\rho} \) by
\[ \Omega_\Sigma = \{ z : \frac{1}{2} \Sigma^{-1} z^2 \leq 1 \} = \{ z : Mz^2 \leq \hbar \} \]
we have the following important geometric reformulation of the quantum condition (60):

**Theorem 5 (Wigner ellipsoid)** The quantum condition \( \Sigma + \frac{i\hbar}{2} J \geq 0 \) is satisfied if and only if \( \Omega_\Sigma \) contains a symplectic ball \( S(B_{2n}^{2\hbar}) \); equivalently
\[ \text{Cap}(\Omega_\Sigma) \geq \pi \hbar \] (62)
where \( \text{Cap}(\Omega_\Sigma) \) is the symplectic capacity [44] of the covariance ellipsoid.

We have given a proof of these properties in [17, 18, 28]; it makes use of the Williamson symplectic diagonalization of \( M \) and essentially consists in showing that the condition (60) is equivalent to the property that the symplectic eigenvalues of \( M = \frac{\hbar}{2} \Sigma^{-1} \) all are \( \leq 1 \). We have called symplectic balls of the type \( S(B_{2n}^{2\hbar}) \) quantum blobs [20]; they appear in the Wigner formalism as minimum uncertainty phase space ellipsoids. The condition (62) can be restated by saying that \( \Omega_\Sigma \) is the Wigner ellipsoid of a Gaussian state if and only if contains a quantum blob.

Summarizing: there is a one-to-one correspondence between phase space ellipsoids \( \Omega_\Sigma \) satisfying \( \text{Cap}(\Omega_\Sigma) \geq \pi \hbar \) and Gaussian states with Wigner ellipsoid \( \Omega_\Sigma \).

\(^7\)It is actually an equivalent form of the Robertson–Schrödinger inequalities [18, 28].
2.3 Time evolution of quantum subsystems

Let \( \hat{\rho} \) be a density matrix on \( \mathbb{R}^n \) with Wigner distribution

\[
\rho(z) = \int_{\mathbb{R}^n} e^{i p \cdot y} \langle x + \frac{1}{2} y | \hat{\rho} | x - \frac{1}{2} y \rangle \, dy .
\]

We assume from now on that \( \rho(z) \) is a Gaussian \((57), (59)\) and, returning to the notation \( z = (z_A, z_B) \), we write \( M = \frac{1}{2} \Sigma^{-1} \) in block-form

\[
M = \begin{pmatrix} M_{AA} & M_{AB} \\ M_{BA} & M_{BB} \end{pmatrix}.
\] (63)

Since \( M = M^T > 0 \) we have \( M_{AA}^T = M_{AA} > 0 \), \( M_{BB}^T = M_{BB} > 0 \), and \( M_{BA}^T = M_{AB} \). We define the Wigner distribution of the subsystem \( A \) by “taking the partial trace”

\[
\rho_A(z_A) = \int_{\mathbb{R}^{2n_B}} \rho(z_A, z_B) \, dz_B .
\] (64)

A straightforward calculation of Gaussian integrals yields the formula

\[
\rho_A(z_A) = (\pi \hbar)^{-n_A} (\det M_{BB})^{1/2} e^{-\frac{1}{\hbar} (M_{BB}) z_A^2}
\] (65)

hence the covariance matrix of \( \rho_A \) is

\[
\Sigma_A = \frac{\hbar}{2} (M_{BB})^{-1}
\] (66)

and the covariance ellipsoid of \( \rho_A \) is thus

\[
\Omega_A = \{ z_A : (M_{BB}) z_A^2 \leq \hbar \} ;
\] (67)

it is the orthogonal projection \( \Pi_A \Omega \) on \( \mathbb{R}^{2n_A} \) of the covariance ellipsoid \( \Omega \) of \( \hat{\rho} \). For \( \rho_A(z_A) \) to qualify as the Wigner distribution of a \( \text{bona fide} \) partial mixed state \( \hat{\rho}_A = \text{Tr}_B(\hat{\rho}) \) it still remains to prove\(^8\) that \( \Sigma_A \) satisfies the quantum condition \((60)\). In view of Theorem \(5\) it suffices for this to show that \( \Omega_A \) contains a symplectic ball \( S_A(B_{\sqrt{\hbar}}) \). But this is an immediate consequence of the extended principle of the symplectic camel in Theorem \(3\) in view of the “only if” part of Theorem \(5\) the covariance ellipsoid \( \Omega_\Sigma \)

\(^8\)This step is usually ignored in the literature. It is needed to show that the partial trace indeed is a positive operator. It can be proven directly using methods from functional analysis (the “Kastler–Loupias–Miracle-Sole conditions). Our approach using the extended PSC is much simpler.
contains a symplectic ball \( S(B_{\sqrt{\hbar}}^{2n}) \) in \( \mathbb{R}^{2n} \) and hence \( \Omega_A = \Pi_A \Omega \) contains a symplectic ball \( S_A(B_{\sqrt{\hbar}}^{2n_A}) \) in \( \mathbb{R}^{2n_A} \).

We apply the results above to the motion of quantum subsystems. We begin by noting that the Wigner transform directly links the approximate Hamiltonian flow \( U_t(z_0) = T(z_t)S_t(z_0)T(-z_0) \)

to the corresponding semiclassical propagator \( \tilde{U}_t(z_0) = e^{i\frac{\gamma(t)}{\hbar}}\tilde{T}(z_t)\tilde{S}_t(z_0)\tilde{T}(-z_0) \)

via the intertwining formulas (50), (51). We have:

\[
W(\tilde{U}_t(z_0)\psi)(z) = W(\psi(U_t(z_0)^{-1}(z))) \quad (68)
\]

Here is a simple proof of this equality. Since the prefactor \( e^{i\frac{\gamma(t)}{\hbar}} \) in \( (47) \) is eliminated by complex conjugation in the definition \( (49) \) of the Wigner transform we have, using several times (50), (51),

\[
W(\tilde{U}_t(z_0)\psi)(z) = W(\tilde{T}(z_t)\tilde{S}_t(z_0)\tilde{T}(-z_0)\psi)(z)
= W(\tilde{S}_t(z_0)\tilde{T}(-z_0)\psi)(z - z_t)
= W(\tilde{T}(-z_0)\psi)(\tilde{S}_t(z_0)^{-1}(z - z_t))
= W\psi(\tilde{S}_t(z_0)^{-1}(z - z_t) + z_0). 
\]

Now, for any \( z \in \mathbb{R}^{2n} \),

\[
U_t(z_0)^{-1}z = T(z_0)S_t(z_0)^{-1}T(-z_t)z
= S_t(z_0)^{-1}(z - z_t) + z_0 
\]

from which the equality in (68) follows.

Let us state and prove our main result. We write \( P_t(z_0) = (S_t(z_0)S_t^T(z_0))^{-1} \)
in block matrix form (33).

**Theorem 6** Assume that the bipartite quantum system \( A \cup B \) is in the Gaussian state \( |\phi_{z_0}\rangle \) at initial time \( t = 0 \):

\[
\phi_{z_0}(x) = (\pi\hbar)^{-n/4}e^{i\rho_0 x}/\hbar e^{-|x-x_0|^2/2\hbar}. 
\]

At time \( t \) the subsystem \( A \) will be in a Gaussian mixed state \( \hat{\rho}_{A,t} \) with Wigner distribution

\[
\rho_{A,t}(z) = (\pi\hbar)^{-n_A}(\det M_A(t,z_0))^{1/2}e^{-\frac{1}{2}M_A(t,z_0)z^2} \quad (69)
\]

20
with

\[ M_{A,t}(z_0) = P_t(z_0)/P_{BB,t}(z_0) \].

The purity of the state \( \hat{\rho}_{A,t} \) is

\[ \mu(\hat{\rho}_{A,t}) = \frac{1}{\sqrt{\det P_{BB,t}(z_0)}}. \]  (70)

**Proof.** It is sufficient to study the case \( z_0 = 0 \) since the general case is obtained by translations. To simplify notation we write \( U_t, P_t, S_t, \) etc. instead of \( U_t(0), P_t(0), S_t(0), \)...

The classical and semiclassical evolution operators are thus here

\[ U_t = T(z_t) + S_t, \quad \hat{U}_t = \hat{T}(z_t) + \hat{S}_t. \]

In the geometric phase space picture \( \phi_{z_0} = \phi_0 \) is represented by the phase space ball \( B_{2^{2n}/\sqrt{\hbar}} \), and we have

\[ U_t = \{ z_t \} + S_t(B_{2^{2n}/\sqrt{\hbar}}) \]

to which corresponds the pure Gaussian state \( \hat{U}_t\phi_0 \). In view of formula (68) we have

\[ W(\hat{U}_t\phi_0)(z) = W\phi_0(U_t^{-1}z). \]  (71)

In view of the extended principle of the symplectic camel, the evolution of the orthogonal projection

\[ \Omega_{A,t} = \Pi_A(U_t(B_{2^{2n}/\sqrt{\hbar}})) \]

on the partial phase space \( \mathbb{R}^{2n_A} \) satisfies

\[ \Omega_{A,t} \supset \{ z_{A,t} \} + S_{A,t}(B_{2^{2n_A}/\sqrt{\hbar}}) \]  (72)

(formula (31) in Theorem 4). It is explicitly given by

\[ \Omega_{A,t} = \{ z_A : (P_t/P_{BB,t})z_A^2 \leq \hbar \} \]

where

\[ P_t/P_{BB,t} = (S_{A,t}^{-1})^T D_{A,t} S_{A,t}^{-1} \]

is the Schur complement of \( P_{BB,t} \) in \( P_t = (S_t S_t^T)^{-1} \). In view of formula (65) \( \Omega_{A,t} \) is the covariance ellipsoid of a mixed quantum state with Wigner distribution

\[ \rho_A(z_A) = (\pi\hbar)^{-n_A} (\det(P_t/P_{BB,t}))^{1/2} e^{-\frac{1}{\hbar}(P_t/P_{BB,t})z_A^2} \]
hence (69). In view of formula (61) the purity of this state is

\[ \mu(\hat{\rho}_{A,t}) = \sqrt{\det(P_t/P_{BB,t})} \]

whence (70) in view of formula (35). ■

Comparing formulas (40) and (70) we see that the variations of classical entropy and mixedness are related by

\[ \Delta S = -2k_B \ln \mu(\hat{\rho}_{A,t}) \]  \hspace{1cm} (73)

As in Section 1.3 (formula (36)) the mixedness of the projected state increases due to its interaction with the subsystem \( B \). It remains constant if and only if \( \hat{\rho}_{A,t} \) is a pure state, which requires, as in the classical case, that \( P_t(z_0) = P_{AA,t}(z_0) \oplus P_{BB,t}(z_0) \) which means that the subsystems \( A \) and \( B \) do not interact.

### 3 Perspectives and Speculations

All our results for subsystems (both classical and semiclassical) crucially depend on the generalization in Theorem 3 to the linear case of Theorem 2 (the principle of the symplectic camel). A natural question that arises is whether one could extend Theorem 3 to more general canonical transformations than the linear (or affine) ones. For instance, if \((\Phi^H_t)\) is the phase-flow determined by a Hamiltonian of the classical type

\[ H(x,p,t) = \frac{1}{2}m^{-1}p^2 + V(x,t) \]

could it be true that the projections of \( \Phi_t(B^{2n}(R)) \) onto the subspaces \( \mathbb{R}^{2n_A} \) and \( \mathbb{R}^{2n_B} \) contain images of the balls \( B^{2n_A}(R) \) and \( B^{2n_B}(R) \) by canonical transformations of \( \mathbb{R}^{2n_A} \) and \( \mathbb{R}^{2n_B} \)? When \( n_A = 1 \) this is trivially true in view of Gromov’s theorem: the projection of \( \Phi_t(B^{2n}(R)) \) onto the plane \( \mathbb{R}^{2n} \) has an area of at least \( \pi R^2 \) and must therefore contain the image of the disk \( B^2(R) \) by an area-preserving diffeomorphism of the plane and such diffeomorphisms are automatically canonical. In the general case \( n_A > 1 \) the problem is open at the time of writing; in fact Abbondandolo and Matveyev [2] have shown that there exist Hamiltonian flows \( \Phi_t \) for which the answer is negative, but the associated Hamiltonians are very unphysical. On the positive side, as already mentioned above, Abbondandolo and Benedetti [1] have recently refined the results in [2] and shown that if the \( \Phi_t \) are sufficiently close to linear canonical transformations, then Theorem 3 applies after some
adequate modifications. Even if it is hard to see why such properties should not be true, we are lacking, for the time being, mathematical justifications; the above mentioned advances are highly qualitative and seem to be difficult to implement in practice. They certainly deserve to be studied further.

Another topic which might be worth exploring using the methods outlined in this paper is the study of Poincaré recurrence for subsystems. As we have explained elsewhere [22] the notion of symplectic capacity seems to play a fundamental role in recurrence (it was one of the motivations of Gromov in his study [29] of symplectic non-squeezing properties). It is clear from Theorem 3 that recurrence in the subsystems $A$ and $B$ is liable to occur faster than in the total system $A \cup B$. It would be interesting to study this property in relation with the entropy briefly discussed in Section 1.3.

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