The quantum canonical ensemble in phase space

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1. Introduction

Nearly a century has passed since Eugene Wigner constructed a representation of the density operator as a real function, which allows for the evaluation of the expectation value of observables as if they were classical phase space averages [1]. The full quantum nature of the Wigner function is given away by the negative values that it assumes for nearly all pure density operators, but the quantum essence of mixed states may not be revealed so explicitly. Indeed, the thermal Wigner function that represents the Gibbs ensemble, or the canonical ensemble, of quantum states in thermal equilibrium with the environment is typically positive, though it leads to strong deviations from a classical average for observables at low temperatures. In the limit of high temperatures, the Wigner function is indistinguishable from its classical counterpart, so the first aim of this paper is to show how quantum corrections creep in as the temperature is lowered. A connection with the underlying classical system is still tenable at temperatures that reach down to the ground state energy, but the semiclassical theory for this, which we here develop, requires either the complexification of the classical Hamiltonian, or the duplication of the real phase space.

The classical canonical ensemble is characterized by the *thermal probability density*: Given the *Hamiltonian*, $H(\mathbf{x})$, for a physical system with N degrees of freedom, defined in the $2N$-dimensional *phase space* with coordinates $\mathbf{x} = (\mathbf{p}, \mathbf{q}) = (p_1, \ldots, p_N, q_1, \ldots, q_N)$, the probability density is

$$P_\beta(\mathbf{x}) \equiv \frac{\exp\{-\beta H(\mathbf{x})\}}{\int \mathrm{d}\mathbf{x}\ \exp\{-\beta H(\mathbf{x})\}}. \tag{1.1}$$

Overall, the classical motion is assumed to be bounded, with an absolute minimum for the Hamiltonian. The only free parameter is $\beta = 1/\kappa_B T$, where T is the temperature and κ_B is Boltzmann's constant. Physically, the thermal distribution results through equilibrium with an external environment, which need not be further invoked here. Since $1/\beta$ is the half-width of the energy distribution, it is evident that $P_\beta(\mathbf{x})$ becomes quite irrelevant for the description of the true physical system, if $\kappa_B T$ is lower than the first excitation energy of the corresponding quantum system.

The *thermal density operator*

$$\hat{\rho}_\beta \equiv \frac{1}{Z_\beta}\ \mathrm{e}^{-\beta\hat{H}}, \tag{1.2}$$

replaces the thermal probability density in the quantum description of the canonical ensemble of states in thermal equilibrium;

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the *partition function* being defined as

$$Z_\beta \equiv \mathrm{tr}\, \mathrm{e}^{-\beta\hat{H}}. \tag{1.3}$$

This is a mixed state of the *eigenstates* $|j\rangle$ of the Hamiltonian $\hat{H}$, which is constrained here only by its energy spectrum, assumed to be discrete, countable and bounded from below. Choosing the sequence of *eigenenergies* E_j to be non-decreasing with the index j, the spectral decomposition,

$$\mathrm{e}^{-\beta\hat{H}} = \sum_j \mathrm{e}^{-\beta E_j}\ |j\rangle\langle j|, \quad Z_\beta = \sum_j \mathrm{e}^{-\beta E_j}, \tag{1.4}$$

reveals that at low temperatures $\hat{\rho}_\beta$ has no relation to the classical distribution $P_\beta(\mathbf{x})$. Instead it is dominated by the ground state $|0\rangle$ and the lowest excited states.

This paper deals exclusively with the equilibrium of quantum systems for which the correspondence principle ascribes a unique classical Hamiltonian as described above. The typical picture corresponds to a few particles or a few degrees of freedom, coupled with a heat bath, and whose Hamiltonian can be developed in the vicinity of one of its critical points.

It is important to note that, even though Planck's constant $\hbar$ does not appear explicitly in (1.2), it fundamentally affects both the eigenstates and the density of states. Indeed, it can be an advantage to consider the non-normalized thermal operator as a continuation of the unitary evolution operator

$$\hat{U}_t = \mathrm{e}^{-it\hat{H}/\hbar} \tag{1.5}$$

for the *imaginary thermal time* $t = -i\theta$ with $\theta = \hbar\beta$. Thus, by formally relaxing β to be positive or negative, these operators also form a group in one-to-one correspondence with the group of unitary evolution operators. There may be no physical relevance for the group properties of the entire set of thermal operators, but Feynman [2] employs their Abelian subgroups, which share the same constant Hamiltonian, to construct path integrals for the thermal operators with finite β.

Of course, Planck's constant is fixed, but the ratio of $\hbar$ to an appropriate action of the system is the standard parameter for semiclassical (SC) approximations to the evolution operator and so it is considered here. There are several methods for the construction of SC approximations, including the stationary phase evaluation of path integrals (see e.g. [3]). It is curious that Feynman never explored these possibilities, neither for the evolution operator, nor as an approximation to the thermal operator, such as presented in [4]. This extension, our present concern, requires attention to the delicate interaction of both parameters, β and $\hbar$. Indeed, it is somewhat paradoxical that one should consider the *thermal time* within the classical Hamiltonian flow itself, even though $\theta = \hbar\beta$, that is, the time which parametrizes the underlying classical motion depends on the fundamental quantum constant.

The standard choice for the investigation of the properties of the density operator is the position representation, that is, the density matrix, as in [2]. Even so, it is the Weyl representation, which best spans the deep gulf between the classical and the quantum regimes. Observables $\hat{O}$ are represented by real functions $O(\mathbf{x})$, which usually equal (or closely approximate) the corresponding classical variable, whereas the density operator is portrayed by the Wigner functions $W(\mathbf{x})$, so as to evaluate the quantum expectation value as

$$\langle\hat{O}\rangle = \mathrm{tr}\ \hat{\rho}\ \hat{O} = \int \mathrm{d}\mathbf{x}\ W(\mathbf{x})\ O(\mathbf{x}). \tag{1.6}$$

For a pure state $|\psi\rangle$ the density operator is the projector, $\hat{\rho} = |\psi\rangle\langle\psi|$, whereas a mixed state is a superposition of projectors onto orthogonal states, weighed by their probability. Given that the identity operator, $\hat{I}$, has the Weyl representation $I(\mathbf{x}) = 1$, so that

$$\langle\hat{I}\rangle = \mathrm{tr}\ \hat{\rho}\ \hat{I} = \int \mathrm{d}\mathbf{x}\ W(\mathbf{x}) = 1, \tag{1.7}$$

the usual convention for the normalization of the Wigner function differs from the Weyl representation of $\hat{\rho}$: $\rho(\mathbf{x}) = (2\pi\hbar)^N W(\mathbf{x})$.

Often, observables correspond closely to classical phase space functions,[1] so that the integral in (1.6) may well wash away detailed oscillatory structures of the Wigner function. But $\hat{O}$ may also stand in for another projector, $|\phi\rangle\langle\phi|$, so that here $\langle\hat{O}\rangle = \mathrm{Pr}(\phi)$, the probability of finding the system in the state $|\phi\rangle$. In particular, for $|\phi\rangle = |\mathbf{X}\rangle$, the *coherent state* centred on the phase space point $\mathbf{X}$, for which

$$W_{\mathbf{X}}(\mathbf{x}) = \frac{1}{(\pi\hbar)^N} \exp\ -\frac{(\mathbf{x}-\mathbf{X})^2}{\hbar}\ , \tag{1.8}$$

so that one can choose $O(\mathbf{x}) = (2\pi\hbar)^N W_{\mathbf{X}}(\mathbf{x})$, the integral for the probability $\mathrm{Pr}(\mathbf{X})$ will pinpoint a classically minute (possibly negative) region of the Wigner function.

Last but not least, the Hermitian reflection operator, around the point $\mathbf{X}$, is given in terms of the vector operator $\hat{\mathbf{x}} = (\hat{\mathbf{p}}, \hat{\mathbf{q}})$ as

$$\hat{R}_{\mathbf{X}} = \int \frac{\mathrm{d}\mathbf{x}}{(4\pi\hbar)^N} \exp\ \frac{i}{\hbar}\mathbf{x}\wedge(\hat{\mathbf{x}}-\mathbf{X})\ , \tag{1.9}$$

introducing the *wedge product* $\boldsymbol{\xi}\wedge\mathbf{x} = (\mathbf{J}\boldsymbol{\xi})\cdot\mathbf{x}$, where the standard symplectic matrix in Hamilton's equations is

$$\mathbf{J} = \begin{matrix} 0 & -1 \\ 1 & 0 \end{matrix} \tag{1.10}$$

in terms of $(\mathbf{p}, \mathbf{q})$ blocks. Also known as the parity operator around $\mathbf{X}$, it is a bona fide observable, experimentally measured in quantum optics [5], and it is the defining operator for the Weyl representation and the Wigner function [6–8][2]:

$$W(\mathbf{X}) \equiv \frac{1}{(\pi\hbar)^N}\ \mathrm{tr}\ \hat{\rho}\ \hat{R}_{\mathbf{X}}. \tag{1.11}$$

The fact that the Wigner function itself may be considered as the average of the parametrized observable $\hat{R}_{\mathbf{x}}$ exemplifies the quantum richness of this seemingly classical phase space representation.

The subject of our study is the *thermal Wigner function*, $W_\beta(\mathbf{x})$, the appropriately normalized Weyl representation of the thermal density operator (1.2). In its spectral decomposition, we then have

$$W_\beta(\mathbf{x}) = \frac{1}{Z_\beta}\sum_j \mathrm{e}^{-\beta E_j}\ W_j(\mathbf{x}), \tag{1.12}$$

where $W_j(\mathbf{x})$ is the pure state Wigner function which represents the eigenstate $|j\rangle$ in phase space. In the following section a schematic overview of the thermal Wigner function discusses the extreme regimes: At very low temperatures energy scales are accessed where it depends only on $\hbar$, whereas one reaches a purely classical dependence on β at very high temperatures. The objective is to present a full SC theory that bridges these regimes. It will be shown that the first simple correction to the high temperature limit depends on a dimensionless parameter, which combines the product of both basic physical parameters, forming the thermal time, together with a further local frequency, given by a local minimum of the classical Hamiltonian.

[1] For the Hamiltonians that follow, we will not distinguish the classical from the Weyl functions.

[2] The review [8] expounds the general background for the interplay of classical and quantum mechanics within SC approximations that is here adapted to the thermal context.

In Section 3, we exploit the direct course of extending analytically the evolution operator within the Weyl representation, i.e. the *Weyl propagator* [8,9], in terms of the imaginary thermal time. This is achieved for quadratic Hamiltonians for which the SC approximation is closed and exact. Not only does this procedure provide the low temperature limit of the thermal Wigner function for a generic Hamiltonian with a quadratic minimum, but a local expansion sheds light on the high temperature limit of the SC approximation. A further employment of analytical continuation in Section 4 also allows for explicit formulae for the SC approximation for a Hamiltonian in its normal form, including the Kerr Hamiltonian [10] as a special case. It should be noted that the exposition up to this section already supplies valuable corrections to the classical high energy approximation, which do not depend on the intricacies of the full SC approximations, which then follow.

The direct course is then to push through the SC approximation of the Wigner function, relying on the trajectories within a complexified phase space, previously developed in the context of the evolution of Markovian quantum systems [11]. This is contained in the recent paper dealing with the SC approximation for the quantum Jarzynski equality [12] and it is not reproduced here. It should be noted that the need of finding classical trajectories, which are only implicitly defined by boundary conditions, faces here the increased difficulty of a search in the complex phase space.

The new development is the expression of the SC Weyl propagator in a doubled real phase space, which proceeds by splitting each classical trajectory into a pair of half trajectories moving backwards and forwards in time. Again, this is also based on a previous SC treatment for the quantum Markovian evolution of the Wigner function [13], but we shall point out important differences involved in this change of context. Presented in Section 5, the ordinary phase space variables, $\mathbf{x} = (\mathbf{p}, \mathbf{q})$, take on the role of *double positions*. To this one adds a $(2N)$-dimensional space of *double momenta*, $\mathbf{y}$, so that the relevant classical motion is generated by a double Hamiltonian $\mathbb{H}(\mathbf{x}, \mathbf{y})$ constructed from $H(\mathbf{x})$. In Section 6 the complexification of time is incorporated within an imaginary double momentum, following which we retrieve a real double phase space. Here the relevant classical motion is generated by a new real double Hamiltonian.

In Section 7 the partition function and the thermal average of an arbitrary observable $\hat{O}$ in (1.6) are then obtained in terms of initial values for the pair of forward and backward trajectories. This eliminates the search for trajectories satisfying implicit boundary conditions, which plagues the practical application of standard SC methods. Saddle point approximations for the partition function and expectations are then considered, pointing to the absence of periodic orbit contributions in the neighbourhood of the minima of the Hamiltonian. Thus, the SC partition function avoids the elaborate resonant structure of the trace of the SC propagator in real time.

The SC scenario in which the thermal Wigner function effects a *pseudo-evolution* in thermal time is then discussed in Section 8. Appendix A presents the SC version of some standard thermodynamic relations and Appendix B discusses the accuracy of the approximation, explicited in the case of a normal form Hamiltonian.

2. Overview of the thermal Wigner function and its parameters

Even though we will not work with the spectral decomposition of the thermal Wigner function directly, it does provide a rough guide to the various regimes. Let us place the absolute minimum of the classical Hamiltonian $H(\mathbf{x})$ at the origin of phase space with $H(0) = 0$. This stable equilibrium has generically the lowest Taylor approximation

$$H(\mathbf{x}|\mathbf{H}) \equiv \frac{1}{2}\, \mathbf{x} \cdot \mathbf{H}\, \mathbf{x}\ , \tag{2.1}$$

a real positive quadratic form defined by the Hessian matrix of the Hamiltonian, whatever the number of degrees of freedom. It will be important here to consider (homogeneous) quadratic Hamiltonians as a class on their own, parametrized by the matrix $\mathbf{H}$. This generates the class of all linear canonical, i.e. *symplectic transformations*.

If $\hbar$ is *small enough*, the lowest eigenenergies lie in the quadratic region and, in the limit of extremely low temperature, the spectral decomposition (1.12) is dominated by the ground state of the quantized version of (2.1). The explicit form of this Wigner function is reduced in the following section to that for a N-dimensional harmonic oscillator, that is, $W_{\mathbf{x}=0}(\mathbf{x})$ in (1.8). Increasing β beyond this point does not affect the thermal Wigner function, which is only parametrized by $\hbar$. On the other hand, if a slight increase of temperature brings in just a few significant states within the spectral decomposition (1.12), while still lying within the quadratic region of the Hamiltonian, these will be *Fock states*, with Wigner functions given by their Grönewold expression [14]

$$W_j(\mathbf{x}) = \frac{(-1)^j}{\pi\hbar} e^{-\mathbf{x}^2/\hbar} L_j\quad \frac{2\mathbf{x}^2}{\hbar}\quad , \tag{2.2}$$

where L_j is the j'th Laguerre polynomial, so that there are concentric positive and negative rings within the quantized energy level. Further decrease of β allows states at higher energy, for which the quadratic approximation of $H(\mathbf{x})$ no longer holds, to participate in the expansion (1.12) for the thermal Wigner function, but an integrable approximation via normal forms can still be quite accurate [15,16]. This is the regime where the SC approximation [17] (see also [18]) constructs each $W_j(\mathbf{x})$, the Wigner function for a (nearly) integrable eigenstate, in terms of the Airy function, enveloping each Bohr-quantized torus. For even smaller β, energies corresponding to a saddle point of $H(\mathbf{x})$ may be accessed, or in any case, chaotic motion may well become prevalent, so that the point is reached where no SC approximation for an individual state is available any longer.

Notwithstanding this basic difficulty, one may still have recourse to Berry's semiclassical approximation for a *microcanonical ensemble of states*, coarse grained over an energy window that is classically very narrow, but which still contains many eigenstates, due to their high semiclassical density [19]. Then one is freed from the details of the classical motion, whether integrable, chaotic or mixed, and the basic feature is a single Airy function that reaches a maximum very near the classical energy shell, decays outside of it and oscillates inside (reaching into a rich structure of caustics [8]). Crudely, this microcanonical Wigner function can be approximated as a Dirac delta-function over the energy shell, which, even so, gives reasonable averages (1.6) for smooth classical observables.

In any case, a general feature is that each contribution to the spectral sum (1.12) hardly affects the thermal Wigner function outside its corresponding energy shell. This indicates that the classical approximation, $W_\beta(\mathbf{x}) \approx P_\beta(\mathbf{x})$ given by (1.1), is at least an envelope for the thermal Wigner function at the high energies accessed by a high temperature. But the same result follows from keeping just the first term in the power expansion of the exponential operator $\exp\{-\beta\hat{H}\}$ in the Weyl representation. Such an expansion requires a high temperature, but the full validity of this approximation will be seen to depend on the smallness of the *thermal time* $\theta = \hbar\beta$, together with a local classical frequency, which will be introduced shortly.

3. Analytic continuation of the Weyl propagator

The quantum flow $\hat{U}_t$ generated by a Hamiltonian $\hat{H}$ may be SC-approximated in terms of the classical canonical flow $\mathbf{x}_- \mapsto \mathbf{x}_+(t)$ generated by the corresponding classical Hamiltonian $H(\mathbf{x})$. The *Weyl propagator*, its Weyl representation, has the SC-approximation [8,9]

$$U_t(\mathbf{x}) \approx \frac{2^N}{|\det(\mathbf{I}+\mathbf{M}_t)|^{1/2}} \exp\ \frac{i}{\hbar}(S_t(\mathbf{x})) \quad , \tag{3.1}$$

in the simplest instance. The geometric part of the *centre (or Weyl) action* $S_t(\mathbf{x})$ is just the symplectic area between a trajectory arc centred on $\mathbf{x}$, that is, with endpoints $\mathbf{x}_\pm$ satisfying $2\mathbf{x} = \mathbf{x}_+ + \mathbf{x}_-$, and its geometric *chord* $\boldsymbol{\xi} = \mathbf{x}_+ - \mathbf{x}_-$, as shown in Fig. 1. From this, one subtracts Et, where $E = H(\mathbf{x}_-) = H(\mathbf{x}_+)$ (and generally $E \neq H(\mathbf{x})$). For short times, it is guaranteed that there exists a single trajectory satisfying the boundary condition. Eventually, the amplitude may become singular (at a caustic); beyond this, there is more than one chord for each centre, so that the propagator becomes a sum over terms like (3.1). Each term then has an extra *Maslov phase* in the exponent, just a multiple of π in the present context [20].

The trajectory $\tilde{\mathbf{x}}(t', \mathbf{x}_-)$, such that for the full interval $\mathbf{x}_+ = \tilde{\mathbf{x}}(t, \mathbf{x}_-)$, is generated by Hamilton's equations

$$\dot{\mathbf{x}} = \mathbf{J}\frac{\partial H}{\partial \mathbf{x}}, \ \text{or} \ \ \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}} \ \text{and} \ \dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}. \tag{3.2}$$

Then the explicit expression for the centre action is

$$S_t(\mathbf{x}) = \int_0^t \tilde{\mathbf{p}}(t', \mathbf{x}_-)\cdot\dot{\tilde{\mathbf{q}}}(t', \mathbf{x}_-)\, \mathrm{d}t' - \mathbf{p}\cdot(\mathbf{q}_+ - \mathbf{q}_-) - tH(\mathbf{x}_-). \tag{3.3}$$

The classical role of the centre action is that of a *generating function* of the canonical transformation $\mathbf{x}^- \mapsto \mathbf{x}^+$, indirectly through [8]

$$\boldsymbol{\xi} = -\mathbf{J}\frac{\partial S_t}{\partial \mathbf{x}} \ \text{ and } \ \mathbf{x}_+ = \mathbf{x} + \frac{\boldsymbol{\xi}}{2}, \ \ \mathbf{x}_- = \mathbf{x} - \frac{\boldsymbol{\xi}}{2}. \tag{3.4}$$

The linear approximation of this transformation near the $\mathbf{x}$-centred trajectory is defined by the *symplectic monodromy matrix* $\mathbf{M}_t$. This has the Cayley parametrization [8]:

$$\mathbf{M}_t = [\mathbf{I} + \mathbf{J}\mathbf{B}_t]^{-1}[\mathbf{I} - \mathbf{J}\mathbf{B}_t], \tag{3.5}$$

in terms of the symmetric Hessian matrix

$$\mathbf{B}_t(\mathbf{x}) \equiv \frac{1}{2}\,\frac{\partial^2 S_t(\mathbf{x})}{\partial \mathbf{x}^2} \tag{3.6}$$

and the identity matrix $\mathbf{I}$. This allows for the alternative form of the SC propagator (3.1) as [8]

$$U_t(\mathbf{x}) \approx |\det(\mathbf{I} \pm \mathbf{J}\mathbf{B}_t(\mathbf{x}))|^{1/2} \ \exp\ \frac{i}{\hbar}(S_t(\mathbf{x})) \quad . \tag{3.7}$$

A fundamental property of the centre action is that it is an odd function of time, that is, $S_{-t}(\mathbf{x}) = -S_t(\mathbf{x})$, since $S_0 = 0$ and the exchange $\mathbf{x}_+ \leftrightarrow \mathbf{x}_-$ merely reverses the sign of $\boldsymbol{\xi}$ in (3.4).[3] It follows from the first of these equations that the local *plane wave approximation* of the action is

$$S_t(\mathbf{x}') \approx S_t(\mathbf{x}) + \boldsymbol{\xi} \wedge (\mathbf{x}' - \mathbf{x}), \tag{3.8}$$

so that $\mathbf{J}\boldsymbol{\xi}(\mathbf{x})/\hbar$ is the *local wave vector* in phase space of the Weyl propagator. The full expansion of the centre action as a power series in time has only odd terms and hence the complexification $S_{it}(\mathbf{x})$ is a purely imaginary function for all real centres, $\mathbf{x}$.

[3] The reversal of $\boldsymbol{\xi}$ and of $S(t)$ with time follows straight from the definition of the chord of a trajectory in phase space. Hence, there is no restriction to the more familiar notion of *time invariance*, which concerns trajectories in configuration space.

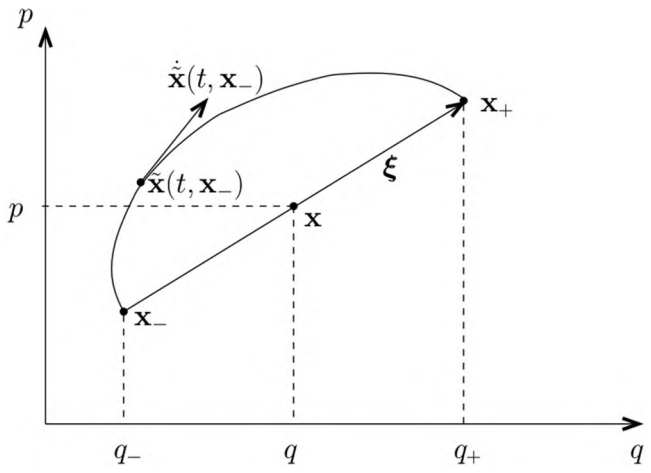

Fig. 1. The action, $S_t(\mathbf{x})$, is just the symplectic area between the trajectory from $\mathbf{x}^-$ to $\mathbf{x}^+$ and its chord $\boldsymbol{\xi}$, from which one subtracts Et, where E is the energy of the trajectory.

The difficulty is that the centre action is not generally expressed as a power series, so that one cannot immediately continue analytically the SC expression $\mathrm{e}^{-\beta H}(\mathbf{x}) \approx U_{-i\hbar\beta}(\mathbf{x})$, in terms of the complex thermal time $t \mapsto -i\hbar\beta = -i\theta$, except in simple cases. In the short time limit, one can neglect the curvature of the trajectory, thus replacing the trajectory arc by the chord itself, whatever the Hamiltonian. In other words, one has $\boldsymbol{\xi} \approx t\dot{\mathbf{x}}$, so that $S_t(\mathbf{x}) \approx -tH(\mathbf{x})$ and $\mathbf{M}_t \approx \mathbf{I}$. For the imaginary thermal time $t = -i\hbar\beta$, one then retrieves the classical high temperature limit of the thermal Wigner function: $W_\beta(\mathbf{x}) \approx P_\beta(\mathbf{x})$.

The Weyl propagator for the harmonic oscillator ($N = 1$)

$$H_h(x) = \frac{\omega}{2}\,(p^2 + q^2) \tag{3.9}$$

provides an illuminating example. After a time t the Cayley matrix for this archetypical elliptic propagator will be $\mathbf{B}_t = -\tan(\omega t/2)\mathbf{I}$ [8,20], so that $S_t(\mathbf{x}) = -\mathbf{x}\cdot\tan(\omega t/2)\mathbf{x}$ and the full Weyl propagator is

$$U_t(\mathbf{x}) = \frac{1}{\cos(\omega t/2)} \exp\ -\frac{i}{\hbar}\tan(\omega t/2)\,(p^2 + q^2) \quad . \tag{3.10}$$

Here, the monodromy matrix, $\mathbf{M}_t$, does not depend on $\mathbf{x}$, leading to the simple form taken by the square root in the amplitude of (3.1). In general, the SC expressions for propagators generated by quadratic Hamiltonians are exact and here it is easy to proceed to the analytic continuation for the imaginary thermal time, $t = -i\theta$. Thus, the exact expression for the Weyl exponential of the Hamiltonian is

$$\mathrm{e}^{-\beta H_h}(\mathbf{x}) = \frac{1}{\cosh(\omega\theta/2)} \exp\ -\frac{1}{\hbar}\tanh(\omega\theta/2)\ (p^2 + q^2) \quad . \tag{3.11}$$

The equality of this analytic continuation of the Weyl propagator with the spectral sum for the thermal Wigner function, summing over the eigenstates given by (2.2), follows simply from the identity:

$$\sum_{j=0}^{\infty} t^j\, L_j(x) = \frac{1}{1-t} \exp\ -\frac{tx}{1-t} \quad , \tag{3.12}$$

with the choice $t = -\exp(-\beta\hbar\omega)$.

One should observe that the Weyl propagator for the inverted harmonic oscillator,

$$H(x) = \frac{\omega}{2}\,(p^2 - q^2), \tag{3.13}$$

is

$$U_t(\mathbf{x}) = \frac{1}{\cosh(\omega t/2)} \exp\ -\frac{i}{\hbar} \tanh(\omega t/2)\,(p^2 - q^2)\ , \qquad (3.14)$$

so that (3.11) is a curious blend of the expressions for the harmonic oscillator and its inverse.[4] In this case, the Hamiltonian can be obtained from a Lagrangian. Its thermal properties are then obtained from the real time propagation in the inverted oscillator [4]. Our treatment of general Hamiltonians in Section 6 may be considered to be a further generalization, since it also replaces a stable equilibrium by an unstable point. First we deal here with the more restricted class of general quadratic Hamiltonians (2.1) and its quantization.

A crucial characteristic of the Weyl representation is its *symplectic invariance*, that is, the functions that represent operators in phase space are invariant under linear canonical transformations of its arguments (see e.g. [18]). Indeed these classical-like transformations are just a particularly apt expression of similarity transformations by the quantum *metaplectic group* of unitary operators [20–22]. These are generated by the quantization of (2.1), such that the SC form is exact, that is, for a single degree of freedom the Weyl propagators for the metaplectic operators are

$$U_t(\mathbf{x}|\mathbf{H}) = \frac{1}{\cos(\Omega t/2)} \exp\ -\frac{1}{\hbar} \tan(\Omega t/2)\, \frac{\mathbf{x}\cdot\mathbf{H}\,\mathbf{x}}{\Omega}\ , \qquad (3.15)$$

where $\Omega^2 \equiv \det \mathbf{H}$.

Thus, the unitary metaplectic operators have the same general form as those which may evolve them through a similarity transformation. This is not so for their analytic continuation as non-normalized thermal Wigner functions, provided $\Omega^2 > 0$. Rather, these *metaplectic Wigner* functions become the exact generalization of (3.11):

$$\mathrm{e}^{-\beta H}(\mathbf{x}|\mathbf{H}) = \frac{1}{\cosh(\Omega\theta/2)} \exp\ -\frac{1}{\hbar} \tanh(\Omega\theta/2)\, \frac{\mathbf{x}\cdot\mathbf{H}\,\mathbf{x}}{\Omega} \qquad (3.16)$$

with $\theta = \hbar\beta$. So one may include, for instance, a constant magnetic field for a charged harmonic oscillator. Extending to $\beta < 0$, the complete set of operators $\exp[-\beta\ \hat{\mathbf{x}}\cdot\mathbf{H}\hat{\mathbf{x}}/2]$ form a group that is isomorphic to the metaplectic group.

In the case of a free particle, such that $\Omega \to 0$ as $\mathbf{x}\cdot\mathbf{H}\,\mathbf{x} \to \mathbf{p}^2/2m$, one obtains

$$\mathrm{e}^{-\beta H}(\mathbf{x}) = \exp\ -\frac{\beta}{2m}\ \mathbf{p}^2\ , \qquad (3.17)$$

a non-normalized version of $P_\beta(\mathbf{x})$. So one encounters the general rule that the Weyl representation of any operator that is a function either exclusively of the momenta, or exclusively of the positions, has exactly its classical form.

For $N > 1$ the transformation which diagonalizes the symmetric matrix $\mathbf{H}$ in the positive quadratic Hamiltonian also places the matrix $\mathbf{JH}$ in its *Williamson normal form* (see e.g. [15]), so that this transformation is symplectic. The only option of the normal form, if the Hamiltonian is bounded from below, is that all degrees of freedom are elliptic. Thus the thermal Wigner function at sufficiently low temperature reduces to a product of N individual harmonic oscillator Wigner functions (3.11) with frequencies ω_n, each in its own phase plane.

The lowest correction to the action for a general Hamiltonian at short times is

$$S_t(\mathbf{x}) \approx -tH(\mathbf{x}) - \frac{t^3}{24}\ \dot{\mathbf{x}}\wedge\ddot{\mathbf{x}} = -tH(\mathbf{x}) - \frac{t^3}{24}\ \dot{\mathbf{x}}\cdot\mathbf{H}_{\mathbf{x}}\,\dot{\mathbf{x}}\ ; \qquad (3.18)$$

[4] Unlike the harmonic oscillator action, which is singular at $\omega t = \pi$, the action for its inverse stabilizes smoothly due to the relevant trajectory merely hugging the stable and the unstable manifold closer and closer as t increases. Due to structural stability, this also holds for nonlinearly deformed unstable equilibria.

the first version derived in [19], whereas the second in [8] evinces the connection with the local quadratic approximation of the Hamiltonian in terms of its Hessian matrix $\mathbf{H}_{\mathbf{x}} = \partial^2 H(\mathbf{x})/\partial\mathbf{x}^2$. Indeed, following the appendix in [8] the local inhomogeneous quadratic approximation to the Hamiltonian

$$H^{(2)}(\mathbf{x}'|\mathbf{x}) \equiv H(\mathbf{x}) + \boldsymbol{h}_{\mathbf{x}}\cdot(\mathbf{x}'-\mathbf{x}) + \frac{1}{2}\,(\mathbf{x}'-\mathbf{x})\cdot\mathbf{H}_{\mathbf{x}}\,(\mathbf{x}'-\mathbf{x}), \qquad (3.19)$$

where $\boldsymbol{h}_{\mathbf{x}}$ is the local gradient of the Hamiltonian, generates a symplectic flow in a kind of tangent space, with points $(\mathbf{x}'-\mathbf{x})$. We can now reexpress this in terms of the homogeneous quadratic Hamiltonian (2.1)

$$H^{(2)}(\mathbf{x}'|\mathbf{x}) = [H(\mathbf{x}) - H(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}}|\mathbf{H}_{\mathbf{x}})] + H(\mathbf{x}'-\boldsymbol{\gamma}_{\mathbf{x}}|\mathbf{H}_{\mathbf{x}}), \qquad (3.20)$$

by defining the local *centre of curvature*:

$$\boldsymbol{\gamma}_{\mathbf{x}} \equiv \mathbf{x} - \mathbf{H}_{\mathbf{x}}{}^{-1}\boldsymbol{h}_{\mathbf{x}}. \qquad (3.21)$$

One should notice that (3.20) holds even for $\mathbf{x}' \to \mathbf{x}$, so that one may evaluate the time derivatives $\dot{\mathbf{x}} = \mathbf{JH}_{\mathbf{x}}(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})$ and $\ddot{\mathbf{x}} = \mathbf{JH}_{\mathbf{x}}\mathbf{JH}_{\mathbf{x}}(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})$ at the centre $\mathbf{x}$ itself. But for a single degree of freedom, $(\mathbf{JH}_{\mathbf{x}})^2 = -\Omega_{\mathbf{x}}^2\mathbf{I}$, so that the acceleration always points to the local centre of curvature: $\ddot{\mathbf{x}} = -\Omega_{\mathbf{x}}^2(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})$.

The quantization of the approximate Hamiltonian (3.20), with $\mathbf{x}$ kept as a constant and further parametrized by the local centre of curvature $\boldsymbol{\gamma}_{\mathbf{x}}$, then identifies the correction to the short time approximation for the centre action (3.18) as merely the third order expansion in time of the action generated by a quadratic Hamiltonian: tan (for real time) and tanh (for imaginary thermal time). For a general Hamiltonian one thus obtains the short time approximation of $\mathrm{e}^{-\beta H}(\mathbf{x})$ as the generalization of the third order expansion of the action in (3.16), i.e.

$$\mathrm{e}^{-\beta H}(\mathbf{x}) \approx \frac{1}{1+(\hbar\beta\Omega_{\mathbf{x}})^2/8} \exp\ -\beta H(\mathbf{x}) - \frac{\hbar^2\beta^3}{24}\ \dot{\mathbf{x}}\cdot\mathbf{H}_{\mathbf{x}}\,\dot{\mathbf{x}} \qquad (3.22)$$

$$= \frac{1}{1+(\hbar\beta\Omega_{\mathbf{x}}/2)^2/2}$$

$$\times \exp\ -\beta H(\mathbf{x}) - \frac{(\hbar\beta\Omega_{\mathbf{x}}/2)^3}{3}\ \frac{(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})\cdot\mathbf{H}_{\mathbf{x}}\,(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})}{\hbar\ \Omega_{\mathbf{x}}}\ .$$

The second form is less convenient for calculations, since it requires the evaluation of the local centre of curvature $\gamma_{\mathbf{x}}$, but it clearly evinces the dimensionless expansion parameter $(\hbar\beta\Omega_{\mathbf{x}}/2)$, where $\hbar\beta = \theta$ is the thermal time, while $\Omega_{\mathbf{x}}$ is the angular frequency of trajectories within the local quadratic approximation.

A final step follows from the recognition that, to be consistent with the local quadratic approximation to the Hamiltonian, one can keep the whole series for tanh and cosh instead of just the third order in the dimensionless parameter. This leads to a dampened version of the metaplectic Wigner function (3.16) with the origin displaced to the centre of curvature $\gamma_{\mathbf{x}}$:

$$\mathrm{e}^{-\beta H}(\mathbf{x}) \approx \mathrm{e}^{-\Delta(\mathbf{x})}\ \ \mathrm{e}^{-\beta H}(\mathbf{x}-\gamma_{\mathbf{x}}|\mathbf{H}_{\mathbf{x}}). \qquad (3.23)$$

The exponent of the attenuation factor in this *local metaplectic Wigner function* is

$$\Delta(\mathbf{x}) = \beta\left(H(\mathbf{x}) - H(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}}|\mathbf{H}_{\mathbf{x}})\right) = \beta H^{(2)}(\gamma_{\mathbf{x}}|\mathbf{x}), \qquad (3.24)$$

so that quantum effects are only represented within the metaplectic Wigner function itself, the second factor in (3.23). One can then picture a tangent space at each point $\mathbf{x}$ as holding a displaced generalized harmonic oscillator, from which the local metaplectic Wigner function is constructed. This alternative form then consists of a classical attenuation of a fully quantum thermal Wigner function, replacing the quantum correction to the classical distribution obtained in (3.22). It is not evident a priori, which of these approximations will best extend to increasing thermal time. One should note that (3.23) is nonsingular for all time, but its real time version will have the singularities of the Weyl propagator for the harmonic oscillator.

4. Normal forms and the Kerr Hamiltonian

For a temperature that includes energies beyond the range of validity of the quadratic approximation, the region surrounding the absolute minimum of the Hamiltonian can be transformed to its *Birkhoff normal form* [15,16], that is, for $N = 1$,

$$H_{Bir}(\mathbf{x}) = \omega \left(\frac{p^2+q^2}{2}\right) + H_2\left(\frac{p^2+q^2}{2}\right)^2 + H_3\left(\frac{p^2+q^2}{2}\right)^3 + \cdots \equiv F\left(\frac{\mathbf{x}^2}{2}\right), \tag{4.1}$$

which simply separates into polynomials $F_n\left(\mathbf{x}_n^2/2\right)$ for higher degrees of freedom. Generally, for $N > 1$, the infinite series has no hope of converging, because the integrable normal form cannot cope with the intricate KAM-type motion that surrounds the equilibrium, but a higher truncation than the simple quadratic can lead to a great improvement in the accuracy of trajectories for a finite time. Evidently this approximation cannot be extended up to a saddle point, if it arises in the Hamiltonian, but the classic expansion by Gustavson [23] for the Hénon–Heiles Hamiltonian [24], below the energy of its three saddles, supplies good trajectories for a finite time.

We cannot use the normal form transformation to transport exactly a Wigner function, because this is a nonlinear transformation, even if it can be chosen to be canonical. Nonetheless, this is just the *truncated Wigner approximation* [25,26] (TWA, also referred to as LSC-IVR [27]). It is widely used and adequate for Wigner functions that are not highly oscillatory, as here, for the Gibbs ensemble. Specially interesting is the *Kerr Hamiltonian*

$$H_K(\mathbf{x}) = \omega \left(\frac{p^2+q^2}{2}\right) + \frac{\omega^2}{\epsilon}\left(\frac{p^2+q^2}{2}\right)^2, \tag{4.2}$$

where ϵ has the dimension of energy, for the single photon Kerr effect [10,28], i.e. simply the harmonic oscillator coupled to its square, so that it arises naturally as an exactly truncated normal form. The quantum evolution of a Kerr system is not governed by an ordinary second order Schrödinger equation, even though its quantum evolution is known exactly [29,30]. The SC treatment relies on a closed expression for the action and, in the case of the homogeneous limit where $\epsilon \to 0$, such that effectively $H_K(\mathbf{x}) \propto H_h(\mathbf{x})^2$, it has been verified in detail [31].

Before considering the analytic continuation of the SC Weyl propagator with an imaginary thermal time for a normal form, let us discuss its fully quantum spectral decomposition in the simple case where $N = 1$. The only dependence on the function F in the definition of the normal form (4.1) lies in the eigenenergies $E_j = F\left(\left(\frac{1}{2}+j\right)\hbar\right)$ determining the weight of the Wigner functions $W_j(\mathbf{x})$ for the eigenstates. That the latter are exactly harmonic oscillator eigenstates is not discrepant with the SC approximation of Berry [17], since it builds each of these Wigner functions relying only on the geometry of the energy level curve, which is here a circle for any form of F.

However, the lowest states are poorly represented by this SC approximation and it is far off from the Gaussian ground state that dominates the thermal Wigner function in the limit of very low temperatures. Indeed, for the exponent in the first term of the spectral sum to be already large, we have $\beta F(\hbar\omega/2) \gg 1$. For a monotonically increasing function F, this would imply that either β or $\hbar$ is large. But for the normal form to be dominated by its first harmonic term, $\hbar$ should be small, as expected within usual SC approximations. Then the condition for the thermal Wigner function to be effectively reduced to that of the harmonic oscillator ground state is expressed in terms of the thermal time as $\theta \gg 2/\omega$. In the extreme case of the homogeneous Kerr system, the correct quantum expression for this low temperature Wigner function still portrays the ground state of the harmonic oscillator, so that correspondence with the classical quartic oscillator is jeopardized.[5]

Even if the energy is too high for individual states to be useful, the normal form may still extend smoothly the picture of the motion beyond the quadratic approximation. For simplicity, the discussion is again limited to a single (typical) degree of freedom. The classical trajectories generated by the normal form are identical to the arcs of concentric circles for the harmonic oscillator, but the angular frequency of each arc depends on its initial value: $\omega(\mathbf{X}) = F'(\mathbf{X}^2/2)$, in terms of the derivative of F with respect to its scalar argument. Let us run forward and backward in time a pair of trajectories from a given point $\mathbf{X}$ for the duration $t/2$. Then the chord joining the endpoints of the full trajectory arc, spanning the angle $tF'(\mathbf{X}^2/2)$, is centred on

$$\mathbf{x} = \cos\left(\frac{t}{2}F'\left(\frac{\mathbf{X}^2}{2}\right)\right)\mathbf{X}. \tag{4.3}$$

The area of the triangle formed by these endpoints with the origin is just $\sin[tF'(\mathbf{X}^2/2)]\,\mathbf{X}^2/2$, which must be subtracted from the arc area $tF'(\mathbf{X}^2/2)\,\mathbf{X}^2/2$ to obtain the area between the trajectory arc and the chord. Finally, subtracting $tH(\mathbf{X}) = tF(\mathbf{X}^2/2)$, one obtains the implicit expression for the action (3.3) as

$$S_t(\mathbf{x}(\mathbf{X})) = tF'\left(\frac{\mathbf{X}^2}{2}\right) - \sin\left(tF'\left(\frac{\mathbf{X}^2}{2}\right)\right)\frac{\mathbf{X}^2}{2} - t\,F\left(\frac{\mathbf{X}^2}{2}\right). \tag{4.4}$$

The analytic continuation of the action for imaginary thermal time $-i\theta = -i\hbar\beta$ is then

$$S_\theta(\mathbf{x}(\mathbf{X})) = \theta F'\left(\frac{\mathbf{X}^2}{2}\right) - \sinh\left(\theta F'\left(\frac{\mathbf{X}^2}{2}\right)\right)\frac{\mathbf{X}^2}{2} - \theta\,F\left(\frac{\mathbf{X}^2}{2}\right). \tag{4.5}$$

The explicit expression obtained by substituting $\mathbf{X}$ by $\mathbf{x}$ is generally much messier but, for the harmonic oscillator one has simply $F' = \omega$, so that only the central term survives and the actions become

$$S_t(\mathbf{x}) = -\tan(t\omega/2)\,\mathbf{x}^2 \quad \text{and} \quad S_\theta(\mathbf{x}) = -\tanh(\theta\omega/2)\,\mathbf{x}^2, \tag{4.6}$$

in line with (3.10) and (3.11).

The amplitude of the thermal Wigner function is again more simply expressed in terms of the centre of the trajectory (see Appendix B):

$$\frac{1}{\cosh\left(\frac{\theta}{2}F'\left(\frac{\mathbf{x}^2}{2}\right)\right)\sqrt{1+\theta\,F''\left(\frac{\mathbf{x}^2}{2}\right)\frac{\mathbf{x}^2}{2}\tanh\left(\frac{\theta}{2}F'\left(\frac{\mathbf{x}^2}{2}\right)\right)}}. \tag{4.7}$$

In practice there is no advantage in working out the full explicit expression for the thermal action in terms of the centre $\mathbf{x}$, since the expectation of observables can be computed by integrating directly over the trajectory midpoint $\mathbf{X}$, as will be discussed in Section 7. On the other hand, it is illuminating to consider the long thermal time limit of $S_\theta(\mathbf{x})$. Recalling the identity $\sinh 2x = 2\sinh x\cosh x$ and that, fixing $\mathbf{x}$, $\mathbf{X} \to 0$ exponentially with increasing thermal time according to the analytic continuation of (4.3), one obtains in the limit a single term

$$S_\theta(\mathbf{x}) \to -\tanh(\hbar\beta F'(0)/2)\,\mathbf{x}^2. \tag{4.8}$$

But $F'(0) = \omega$, so that the SC approximation for the normal form collapses into the thermal Wigner function for the harmonic oscillator just as discussed above. The case of the homogeneous Kerr

[5] One should note that no such prevalence of the ground state arises in the spectral decomposition of the evolution operator in real time, because the weight of each state is just a phase factor.

Hamiltonian is anomalous, since there is no limiting quadratic behaviour.

One should contrast this straightforward SC scenario of the thermal Wigner function for the normal form with the one for the Weyl propagator. The latter has singularities in its action (4.4) and the amplitude of the SC propagator, i.e. *caustics*, which are not a feature of the exact quantum propagator. They subdivide the phase space into distinct regions to be traversed with caution, as exemplified in the case of the Kerr Hamiltonian in [31]. Thus, in comparison, the thermal Wigner function is remarkably well behaved for Hamiltonians with a single minimum. See Appendix B.

The further pursuit of analytic continuation of the classical centre action for general Hamiltonians would be an uncertain enterprise, due to the reliance on approximately integrated trajectories. We henceforth embark on the alternative adaptation of the SC approximation directly to the thermal context. In passing, it should be recalled that for ordinary Hamiltonians, with both the classical and the Weyl form

$$H_s(\mathbf{x}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}), \tag{4.9}$$

the classical dynamical system can be derived directly from a Lagrangian function. This allows for a remarkable simplification of the thermal density matrix in the position representation, through the expedient of redefining the momenta: Imaginary time entails an imaginary velocity in the Lagrangian [4] and hence one deals with *imaginary momentum* $\mathbf{p}^i$ in the Hamiltonian, such that $i\mathbf{p}^i \equiv \mathbf{p}$, so that the only vestige of the complexification is that $\mathbf{p}^2 \mapsto -(\mathbf{p}^i)^2$.[6] This turns stable equilibria into unstable points and vice versa, generalizing the outcome for the harmonic oscillator. Our purpose here is to mimic such a procedure for the Lagrangian, but through a complexification of phase space variables for arbitrary Hamiltonians, so as to obtain a general real SC approximation for the thermal Wigner function.

5. Double phase space

The simple artefact of defining an imaginary momentum does not guarantee that trajectories centred on arbitrary phase space points will be real, even for Hamiltonians of the form (4.9). Nonetheless, the doubling of the phase space does allow for an analogous procedure for general Hamiltonians. Let us first describe this for the Weyl propagator, by breaking up the quantum evolution operator into half-times:

$$\mathrm{e}^{-it\hat{H}/\hbar} = \mathrm{e}^{-it\hat{H}/2\hbar}\,\hat{\mathbf{I}}\,\mathrm{e}^{-it\hat{H}/2\hbar} = \mathrm{e}^{-it\hat{H}_+/2\hbar}\,\hat{\mathbf{I}}\,\mathrm{e}^{+it\hat{H}_-/2\hbar} \tag{5.1}$$

with $\hat{H}_\pm = \pm\hat{H}$. In this last form, one immediately recognizes the operator $\hat{I}_L(t)$, which propagates the *quantum Loschmidt echo or the fidelity*, that is, the overlap of two different evolutions of the same initial state [32]. In the present particular case the pair of quantum evolutions are merely the forward evolution in the interval $(0, t/2)$ and its time reversal $(0, -t/2)$ with the same Hamiltonian $\hat{H}$.

The corresponding classical echo matches the outcome of the following procedure: One picks a real initial value $\mathbf{X}$ and evolves this forwards and backwards in time, $0 \le t' \le t/2$, forming the trajectories $\tilde{\mathbf{x}}_+(\mathbf{X}, t')$ and $\tilde{\mathbf{x}}_-(\mathbf{X}, -t')$. One can then picture the centre and the chord, defined in (3.4), as having evolved continuously in time, from the initial conditions $\tilde{\mathbf{x}}(0) = \mathbf{X}$ and $\tilde{\boldsymbol{\xi}}(0) = 0$ respectively, so that

$$\tilde{\mathbf{x}}(t') = \frac{\tilde{\mathbf{x}}_+(t') + \tilde{\mathbf{x}}_-(t)}{2}\,, \quad \tilde{\boldsymbol{\xi}}(t') = \tilde{\mathbf{x}}_+(t') - \tilde{\mathbf{x}}_-(t'), \quad \text{or} \tag{5.2}$$

$$\tilde{\mathbf{x}}_\pm(t') = \tilde{\mathbf{x}}(t') \pm \frac{\tilde{\boldsymbol{\xi}}(t')}{2}.$$

[6] The switch $\dot{\mathbf{q}}^2 \mapsto -(\dot{\mathbf{q}}^i)^2$ in the Lagrangian is already a part of Feyman's adaptation of the path integral for the density matrix, though the SC limit is not considered in [2].

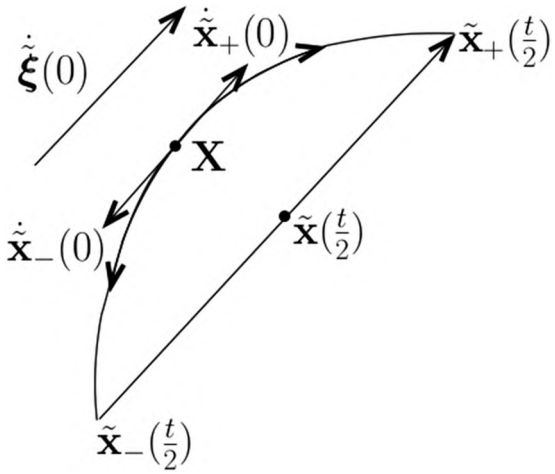

Fig. 2. The action for a doubled time, $S_{2t}(\mathbf{x}(\mathbf{X}))$, is now built up from the forward and backward trajectories, with $\mathbf{X}$ as their initial value.

Then one obtains the action in (3.3) as simply

$$S_t(\mathbf{x}(\mathbf{X})) = \int_0^{t/2} \mathrm{d}t'\; \tilde{\boldsymbol{\xi}}(t') \wedge \dot{\tilde{\mathbf{x}}}(t') - tH(\mathbf{X}), \tag{5.3}$$

At this stage, it is advantageous to define a new variable $\mathbf{y} \equiv \mathbf{J}\boldsymbol{\xi}$. This is the true conjugate variable to $\mathbf{x}$ in the *double phase space* that arises in the semiclassical theory of open quantum systems [11] and superoperators [33]. In this expanded classical picture $\mathbf{x} = (\mathbf{p}, \mathbf{q})$ stands for a *double position*, whereas $\mathbf{y} = (\mathbf{y_p}, \mathbf{y_q})$ assumes the role of its canonical *double momentum*. Thus, the wedge product in (5.3) reduces to an ordinary dot product. Furthermore, it is now possible to define the *double Hamiltonian*

$$\mathbb{H}(\mathbf{x}, \mathbf{y}) \equiv H_+(\mathbf{x} - \frac{\mathbf{Jy}}{2}) - H_-(\mathbf{x} + \frac{\mathbf{Jy}}{2}) = H(\mathbf{x}_+) + H(\mathbf{x}_-) \tag{5.4}$$

such that Hamilton's equations in the enlarged phase space provide the appropriate equations of motion for the centre and chord trajectories in (5.3):

$$\frac{\partial \mathbb{H}}{\partial \mathbf{x}} = \frac{\partial H_+}{\partial \mathbf{x}_+} - \frac{\partial H_-}{\partial \mathbf{x}_-} = -\mathbf{J}(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-) = -\mathbf{J}\dot{\boldsymbol{\xi}} = -\dot{\mathbf{y}} \tag{5.5}$$

$$\frac{\partial \mathbb{H}}{\partial \mathbf{y}} = \frac{\mathbf{J}}{2}\frac{\partial H_+}{\partial \mathbf{x}_+} + \frac{\mathbf{J}}{2}\frac{\partial H_-}{\partial \mathbf{x}_-} = \frac{\dot{\mathbf{x}}_+ + \dot{\mathbf{x}}_-}{2} = \dot{\mathbf{x}}.$$

One should comment that the equalities for both $\dot{\boldsymbol{\xi}}$ and $\dot{\mathbf{x}}$ may seem to subvert intuition for chords and centres for a single evolution generated by $H(\mathbf{x})$, but they are the consequence of taking $H_-(\mathbf{x}) = -H_+(\mathbf{x}) = -H(\mathbf{x})$. Just consider that, for the initial point $\tilde{\mathbf{x}}_+(0) = \tilde{\mathbf{x}}_-(0) = \mathbf{X}$, one has $\dot{\boldsymbol{\xi}} = \dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_- = 2\dot{\mathbf{X}}$, whereas $\dot{\mathbf{x}} = (\dot{\mathbf{x}}_+ + \dot{\mathbf{x}}_-)/2 = 0$ as depicted in Fig. 2. Nonetheless, $\dot{\mathbf{x}}$ is only instantaneously zero, so that $\tilde{\mathbf{x}}(t')$ is not constant, because generally the curvature of the trajectory is nonzero.[7] In conclusion, the double Hamiltonian allows us to express the action in its standard form, as an integral involving the (double) position $\mathbf{x}$ and its conjugate (double) momentum $\mathbf{y}$, evaluated on half the time interval:

$$S_t(\mathbf{x}(\mathbf{X})) = \int_0^{t/2} \mathrm{d}t'\; \tilde{\mathbf{y}}(t') \cdot \dot{\tilde{\mathbf{x}}}(t') - \frac{t}{2}\mathbb{H}(\mathbf{X}). \tag{5.6}$$

The fact that the action is determined by the trajectory midpoint, $\mathbf{X}$, and is here dependent only indirectly on the centre, $\mathbf{x}$,

[7] In previous definitions of a double Hamiltonian [11,13], $\mathbf{y} = 0$ was an invariant plane, but not so here.

may seem to be a disadvantage. On the contrary, it allows us to dispense completely with the *root search* for trajectories in important applications. Indeed differentiating the first equation in (5.2) leads to

$$\frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{X}}(t/2) = \frac{1}{2}(\mathbf{M}_{t/2} + \mathbf{M}_{-t/2}), \tag{5.7}$$

so that, recalling that $\mathbf{M}_{-t} = (\mathbf{M}_t)^{-1}$ and that $\det \mathbf{M}_t = 1$ for all t, the Jacobian determinant for the change of variables $\mathbf{X} \to \tilde{\mathbf{x}}(t/2) = \mathbf{x}$ is

$$|\det \frac{\partial \mathbf{x}}{\partial \mathbf{X}}| = \frac{1}{2^{2N}} \, |\det(\mathbf{I} + \mathbf{M}_t)|. \tag{5.8}$$

But this is just the square of the inverse amplitude of the Weyl propagator (3.1)!

Let us consider the overlap of an initial function $|\psi\rangle$ with its evolution $|\psi_t\rangle = \hat{U}_t|\psi\rangle$. In terms of the corresponding Wigner function $W_\psi(\mathbf{X})$, the exact expression is

$$\langle\psi|\psi_t\rangle = \mathrm{tr}\, \hat{U}_t|\psi\rangle\langle\psi| = \int \mathrm{d}\mathbf{x}\, W_\psi(\mathbf{x})\, U_t(\mathbf{x}). \tag{5.9}$$

Hence, the change of variable $\mathbf{x} \to \mathbf{X}$ leads to the SC approximation

$$\langle\psi|\psi_t\rangle \approx \int \mathrm{d}\mathbf{X}\, |\det \frac{\partial \mathbf{x}}{\partial \mathbf{X}}|^{1/2} \exp\left[\frac{i}{\hbar}(S_t(\mathbf{x}(\mathbf{X}))\right] \quad W_\psi(\mathbf{x}(\mathbf{X}))\,. \tag{5.10}$$

There is no extra integration and no worry about amplitude singularities at caustics, because these are cancelled by the new Jacobian factor in the integral. In this way there is no search for trajectories, even though the Weyl propagator itself is not an *initial value representation* (IVR), such as for instance the Herman–Kluk propagator [27,34]. One should note that previous treatments of time evolution of overlaps within the Weyl–Wigner representation [35] dealt only with its square-modulus, that is, the self correlation of the evolved state.

6. Complexified and decomplexified double phase space

The complexification of time as $t \mapsto -i\hbar\beta$, which has been adopted so far, leads to results that are equivalent to choosing the real *thermal time*, $\theta \equiv \hbar\beta$, together with the complex Hamiltonian

$$H^i(\mathbf{x}) \equiv -iH(\mathbf{x}). \tag{6.1}$$

This is imaginary for real $\mathbf{x}$, so that then $\dot{\mathbf{x}}$ is imaginary and all trajectories depart from the real plane. Such an option is verified to be legitimate in the short time limit of the action (3.18) and one can always build the actions for longer times from the short time trajectory segments [8]. In other words, whereas the SC approximation for the Weyl propagator results from a formally exact path integral by stationary phase integration, its analytic continuation, which we now present, follows from the saddle point approximation to the same path integral with imaginary time. The essential common feature is that the action defined in terms of the set of paths, which share the given centre $\mathbf{x}$, is stationary for classical trajectories.

For a general point in the complex phase space $\mathbf{x} \to \boldsymbol{z}$, Hamilton's equations become

$$\dot{\boldsymbol{z}} = \mathbf{J}\frac{\partial H^i}{\partial \boldsymbol{z}} = -i\mathbf{J}\frac{\partial H}{\partial \boldsymbol{z}}. \tag{6.2}$$

Evaluated at the complex conjugate point $\boldsymbol{z}^*$, one obtains $\dot{\boldsymbol{z}}(\boldsymbol{z}^*) = -[\dot{\boldsymbol{z}}(\boldsymbol{z})]^*$, which is the velocity for the reverse trajectory in time, leading in particular to an imaginary velocity whenever $\boldsymbol{z} = \boldsymbol{z}^*$. Reiterating the process, $\ddot{\boldsymbol{z}}(0)$ will be real, and, more generally, the odd time derivatives will be imaginary whereas the even ones will be real. As a consequence, if we evolve the real phase space point $\mathbf{X}$ forwards and backwards in time, $0 \le \theta' \le \theta/2$, forming the trajectories $\tilde{\boldsymbol{z}}(\mathbf{X}, \theta') = \boldsymbol{z}(0) + \theta\dot{\boldsymbol{z}}(0) + \frac{\theta^2}{2}\ddot{\boldsymbol{z}}(0) + \cdots$ and $\tilde{\boldsymbol{z}}(\mathbf{X}, -\theta') = \boldsymbol{z}(0) - \theta\dot{\boldsymbol{z}}(0) + \frac{\theta^2}{2}\ddot{\boldsymbol{z}}(0) + \cdots$, then $\tilde{\boldsymbol{z}}(\mathbf{X}, -\theta') = [\tilde{\boldsymbol{z}}(\mathbf{X}, \theta')]^*$ and one can define the evolving chord and centre:

$$\begin{cases} \tilde{\mathbf{x}}(\mathbf{X}, \theta') = \dfrac{\tilde{\boldsymbol{z}}(\mathbf{X}, \theta') + \tilde{\boldsymbol{z}}(\mathbf{X}, -\theta')}{2} = \mathrm{Re}\ \tilde{\boldsymbol{z}}(\mathbf{X}, \theta') = \mathbf{x}^r \\ \tilde{\boldsymbol{\xi}}(\mathbf{X}, \theta') = \tilde{\boldsymbol{z}}(\mathbf{X}, \theta') - \tilde{\boldsymbol{z}}(\mathbf{X}, -\theta') = 2i\ \mathrm{Im}\ \tilde{\boldsymbol{z}}(\mathbf{X}, \theta') = -i\boldsymbol{\xi}^i, \end{cases} \tag{6.3}$$

where $\mathbf{x}^r$ and $\boldsymbol{\xi}^i$ are real. Thus, one guarantees that the evolving centre trajectory remains real for all time, whereas the chord is always imaginary. But this is just what one should obtain from the complexification of the time in (3.4): the action being an odd function of time, it becomes purely imaginary for imaginary time and the chord must follow suit.

This preliminary remark sets up the option to map the complexified double phase space into a real double phase space. Assuming analyticity of the action with respect to time, we extend the expression (5.6) to an imaginary time $t = -i\theta$, with $\theta \in \mathbb{R}$, and write

$$S_{-i\theta}(\mathbf{x}(\mathbf{X})) = \int_0^{-i\theta/2} \mathrm{d}t'\ \tilde{\mathbf{y}}(t') \cdot \dot{\tilde{\mathbf{x}}}(t') - \frac{-i\theta}{2}\mathbb{H}(\mathbf{X}, 0), \tag{6.4}$$

with the complex time generalization of (5.6),

$$\begin{cases} \mathbf{y}(0) = 0 \\ \mathbf{x}(0) = \mathbf{X} \\ \dfrac{d\mathbf{y}}{d(-i\theta)} = -\dfrac{\partial \mathbb{H}}{\partial \mathbf{x}}(\mathbf{x}, \mathbf{y}) \\ \dfrac{d\mathbf{x}}{d(-i\theta)} = \dfrac{\partial \mathbb{H}}{\partial \mathbf{y}}(\mathbf{x}, \mathbf{y}). \end{cases} \tag{6.5}$$

The preliminary remark suggests the replacement of $\mathbf{x}$ by $\mathbf{x}^r$ and $\mathbf{y}$ by $-i\mathbf{y}^i$, leading to

$$\begin{cases} \mathbf{y}^i(0) = 0 \\ \mathbf{x}^r(0) = \mathbf{X} \\ \dfrac{d\mathbf{y}^i}{d\theta} = -\dfrac{\partial \mathbb{H}^r}{\partial \mathbf{x}}(\mathbf{x}^r, \mathbf{y}^i) \\ \dfrac{d\mathbf{x}^r}{d\theta} = \dfrac{\partial \mathbb{H}^r}{\partial \mathbf{y}^i}(\mathbf{x}^r, \mathbf{y}^i). \end{cases} \tag{6.6}$$

with

$$\mathbb{H}^r(\mathbf{x}^r, \mathbf{y}^i) = \mathbb{H}(\mathbf{x}, \mathbf{y}) = H(\mathbf{x}^r + i\frac{\mathbf{J}\mathbf{y}^i}{2}) + H(\mathbf{x}^r - i\frac{\mathbf{J}\mathbf{y}^i}{2}). \tag{6.7}$$

Notice that $\mathbb{H}^r(\mathbf{x}^r, \mathbf{y}^i)$ is real if $\mathbf{x}^r$ and $\mathbf{y}^i$ are real, and therefore, since $\mathbf{x}^r$ and $\mathbf{y}^i$ are initially real, Eqs. (6.6) ensure that they will stay real for any θ, thus confirming the preliminary remark.

In its essence, the scenario depicted here is equivalent to our previous treatment of the complex action [12], but it is worth investigating it further. The full trajectory in double phase space may be considered as combining both segments of $\tilde{\boldsymbol{z}}(\mathbf{X}, \pm\theta')$ with $\theta' \ge \frac{\theta}{2}$, or, which is equivalent, the single phase space trajectory $\tilde{\boldsymbol{z}}(\boldsymbol{z}_-, \theta')$, with $\theta' \ge \theta$, generated by $H^i(\boldsymbol{z})$, starting at $\boldsymbol{z}_-$ up to $\mathbf{X}$, and then on to its final point: $\tilde{\boldsymbol{z}}(\boldsymbol{z}_-, \theta) = \boldsymbol{z}_+$. The real part of this trajectory is just $\mathbf{x}^r(\theta/2 - \theta')$ from $\mathbf{x}(\mathbf{X})$ to $\mathbf{X}$ and then it exactly retraces itself, whereas the imaginary part is $J\mathbf{y}^i(\theta/2 - \theta')/2$. This simple behaviour is not the general rule for arbitrary initial points $\boldsymbol{z}_-$, so that it is an asset to be able always to start instead at the real midpoint, $\mathbf{X}$.

With these new real variables, one can see explicitly that the action (6.4) is purely imaginary, that is

$$S_\theta(\mathbf{x}(\mathbf{X})) = (-i)S^i_\theta(\mathbf{x}(\mathbf{X})) \tag{6.8}$$

where the real action $S^i_\theta(\mathbf{x}(\mathbf{X}))$ is defined by

$$S^i_\theta(\mathbf{x}(\mathbf{X})) = \int_0^{\theta/2} \mathrm{d}\theta'\ \mathbf{y}^i(\theta')\cdot\dot{\mathbf{x}}^r(\theta') - \frac{\theta}{2}\mathbb{H}(\mathbf{X},0). \tag{6.9}$$

In other words, the actual exponent of the thermal Wigner function is $S^i_\theta(\mathbf{x}(\mathbf{X}))/\hbar$, and it is built on the dynamics of a trajectory in the real phase space $(\mathbf{x}^r,\mathbf{y}^i)$, so that here $\mathbf{x}^r$ is the generalized position and $\mathbf{y}^i$ is the generalized momentum. Even so, it should be recalled that the double Hamiltonian is entirely specified by $H(\mathbf{x})$ and $\mathbb{H}^r(\mathbf{X},0) = 2H(\mathbf{X})$. Viewed as a function of the centre $\mathbf{x}$, rather than the midpoint $\mathbf{X}$ of the full trajectory generated by the double Hamiltonian $\mathbb{H}^r(\mathbf{x}^r,\mathbf{y}^i)$, one should note that $S^i_\theta(\mathbf{x})$ is exactly portrayed by (3.3), so that this trajectory satisfies the *centre variational principle* [8,36]: In short, the action is stationary with respect to infinitesimal changes of the path in phase space, which preserve its centre $\mathbf{x}$ (as opposed to the trajectory midpoint $\mathbf{X}$).

As an example to help overcome the unfamiliarity of these double phase space expressions, let us return to the simple harmonic oscillator. Feeding its Hamiltonian (3.9) into the general expression for the double Hamiltonian (6.7), while leaving aside the labels ^{r} and ^{i} to alleviate notation, leads to

$$\begin{aligned}\mathbb{H}^r_h(\mathbf{x},\mathbf{y}) &= \omega\quad \mathbf{x}^2 - \Big(\frac{\mathbf{y}^2}{4}\\ &= -\omega\quad \frac{y_p^2}{4} - p^2\Big) - \omega\quad \frac{y_q^2}{4} - q^2\Big),\end{aligned} \tag{6.10}$$

recalling that here one interprets the centre, $\mathbf{x} = (p,q)$, as a double phase space position, whereas the (rotated) chord, $\mathbf{y} = (y_p, y_q)$, stands for the momentum. So we recognize that (6.10) is akin to the Hamiltonian for a double inverted oscillator (3.13) (moving backwards). Resolution of (6.6) gives $\mathbf{x}(\mathbf{X},\theta) = \cosh(\omega\theta/2)\,\mathbf{X}$ and brings the harmonic oscillator action (4.6).

The close connection established in Section 2 between the thermal Wigner function for the harmonic oscillator and the third order short time approximation for general Hamiltonians clearly implies that one can also generalize the procedure above, so as to obtain this approximation within the double phase space approach. Indeed, it is interesting that the original derivation in [19] for the Weyl propagator already makes use of a construction around the midpoint of the trajectory at $t/2$, here labelled $\mathbf{X}$.

A further example of a double Hamiltonian is obtained for the Kerr system (4.2), for which $\mathbb{H}^r_K(\mathbf{x},\mathbf{y}) \neq [\mathbb{H}^r_h(\mathbf{x},\mathbf{y})]^2$. Indeed, in the homogeneous limit of small

$$\begin{aligned}\mathbb{H}^r_K(\mathbf{x},\mathbf{y}) = \frac{\omega^2}{2\epsilon}\Big[&\Big(p^2 - \frac{y_p^2}{4}\Big)^2 + \Big(q^2 - \frac{y_q^2}{4}\Big)^2\\ &+2\Big(p^2 - \frac{y_p^2}{4}\Big)\Big(p^2 - \frac{y_p^2}{4}\Big) - (qy_p - py_q)^2\Big],\end{aligned} \tag{6.11}$$

which has a nonquadratic equilibrium at the origin. In spite of the increased complexity, note that $\mathbb{H}^r_K(\mathbf{x},\mathbf{y}) = 0$ along $\mathbf{x} = \pm\mathbf{y}$, so preserving something of the hyperbolic structure of $\mathbb{H}^r_h(\mathbf{x},\mathbf{y})$.

7. Traces, averages and saddle points

It is important to realize that the explicit action in terms of the trajectory midpoint $\mathbf{X}$, instead of the centre $\mathbf{x}$ at which the thermal Wigner function is evaluated, is no drawback for the evaluation of thermal averages. Indeed, the only difference with respect to the previous case of the wave function overlap at the end of Section 5 is that the real double Hamiltonian, which generates the classical trajectories for the real thermal time $\theta = \hbar\beta/2$ is expressed as (6.7), instead of (5.4). Hence, the same change of integration variable, $\mathbf{x} = \tilde{\mathbf{x}}(\theta/2) \to \mathbf{X}$ with Jacobian (5.8), allows for the full semiclassical thermal average of an arbitrary observable $\hat{O}$ to be expressed as a simple modification of (5.10):

$$\langle\hat{O}\rangle_\beta \approx \frac{1}{Z_\beta}\int \mathrm{d}\mathbf{X}\ |\det\frac{\partial\mathbf{x}}{\partial\mathbf{X}}|^{1/2}\ \exp\ \frac{1}{\hbar}(S^i_{\hbar\beta}(\mathbf{x}(\mathbf{X})))\quad O(\mathbf{x}(\mathbf{X})). \tag{7.1}$$

Here, the partition function Z_β is evaluated by a similar integral in which $O(\mathbf{x}) = 1$. For high temperatures corresponding to short imaginary times there will be no caustics, but even if these should arise, they would only be zero curves, or more general zero manifolds, of the Jacobian determinant. Should they arise, the residual task is then to evaluate an overall sign, which is the only remnant of *Maslov phases* in the Weyl propagator [20] if caustics separate the domain of integration.

The expectation of functions of the energy itself $\langle F(\hat{H})\rangle_\beta$ are important examples of the general SC formula (7.1). They are related by standard thermodynamical relations, which are not quite obvious within the SC approximation, as we discuss in Appendix A.

The exact expression (3.11) supplies the partition function for the harmonic oscillator:

$$\begin{aligned}Z_\beta &= \int \mathrm{d}\mathbf{x}\ \mathrm{e}^{-\beta H}(\mathbf{x})\\ &= \frac{1}{\cosh(\hbar\beta\omega/2)}\int \mathrm{d}\mathbf{x}\ \exp\ -\frac{1}{\hbar}\tanh(\hbar\beta\omega/2)\ (p^2+q^2)\\ &= \frac{\pi\hbar}{\sinh(\hbar\beta\omega/2)}.\end{aligned} \tag{7.2}$$

This diverges for $\beta \to 0$ as the classical high temperature approximation $Z_\beta = 2\pi/\beta\omega$, but then it decays exponentially. Being that the exponent of the thermal Wigner function for the harmonic oscillator is already quadratic, one may identify the above partition function with its own saddle point approximation. For a general Hamiltonian, the validity of this approximation depends on large β so as to confine the thermal Wigner function close to the saddle point at the origin, just the opposite of the high temperature approximation. But this is just the condition for the normal form approximation for the thermal Wigner function in Section 4 to hold, so that it merely collapses onto the central harmonic oscillator.

There is no saddle point contribution to the trace from periodic orbits in the classical flow generated by the hyperbolic double Hamiltonian (6.10), except for the equilibrium point at the origin itself. For the normal form approximation in Section 4 the same is true. A saddle point evaluation of the expectation of an observable, $\hat{O}$, according to (7.1), would be merely $O(0)$, its Weyl value at the origin, which is obviously unsatisfactory at high temperatures, for which the thermal Wigner function is not concentrated near the origin.

Thus, in the limit of low temperatures, one loses the complexity of the full semiclassical theory of the thermal Wigner function when evaluating the thermal average of smooth observables. It is required that the energy has a minimum for any thermal average even to be considered. Then this minimum will correspond generically to an elliptic equilibrium, whatever the number of degrees of freedom; the linearization of the flow (the quadratic approximation of the Hamiltonian) close to this origin provides a (multidimensional) harmonic oscillator. The corresponding double Hamiltonian will then be a (multidimensional) inverted harmonic oscillator, so that we are guaranteed the absence of any periodic orbits in the saddle point approximation of the trace, or the expectation of any smooth observable.

The special case of the Kerr Hamiltonian (4.2) reminds us that there may be no quadratic approximation in the homogeneous limit, but still there is a minimum. In this case, the high

temperature approximation is

$$Z = \int \mathrm{d}\mathbf{x}\ \exp\{-\beta[(\omega/2)\,(p^2+q^2)]^2\} = \frac{\pi}{\omega}\sqrt{\frac{\pi}{\beta}}. \tag{7.3}$$

In contrast, the equilibrium of the quartic double Hamiltonian (6.11) is not a minimum (or maximum), just as that of a hyperbolic Hamiltonian, so that even in this special case there are no periodic orbits, which could contribute to the semiclassical partition function.

Further results on the partition function for the Kerr Hamiltonian are presented in Appendix B.

8. Discussion

The density operator is the appropriate description of a system that is not isolated. Indeed, a system described by an initially pure state, the projector corresponding to a vector in Hilbert space, is known to evolve into a mixed state, losing quantum coherence due to contact with an external environment. Once the equilibrium of the system with the environment is achieved, it is characterized by the overall temperature $T = 1/\kappa_B\beta$, so that the resulting mixed state can be identified with the one defined by the canonical ensemble, provided that the coupling to the environment is sufficiently weak.

The observation that the product $\hbar\beta \equiv \theta$ has the dimension of time, a *thermal time*, permits an analogy of the static thermal density operator to the outcome of a *pseudo-evolution* in θ. The semiclassical approximation of the thermal Wigner function breathes life into this metaphor, with the added quirk that one moves in thermal time from the initial classical canonical distribution, with no trace of Planck's constant, into the quantum realm.

Hamilton's equations and the entire classical pseudo-motion, on which the SC approximation is based, are parametrized by thermal time. For small θ, the classical trajectories are short, so that the semiclassical approximation depends only on a local quadratic approximation of the Hamiltonian. This provides the lowest quantum corrections to the high temperature limit. Increasing thermal time requires the action of a longer trajectory, either immersed in a complexified phase space [12], or in the real doubled phase space presented here. The fact that the appropriate double Hamiltonian has a saddle point instead of a stable equilibrium prevents the relevant trajectory from growing beyond the constraint provided by the pair of stable and unstable manifolds. This limits the action, which converges for large θ to the exponent of the Wigner function of the dominant ground state in the low temperature limit. Therefore our semiclassical approximation bridges the entire range, effectively anchored at both the very high and the very low temperatures. It remains to verify computationally how well it behaves in the intermediate temperature range, that is, intermediate thermal time, given that physically $\hbar$ is a constant.

Having indulged in the metaphor of a *thermal–dynamical* system, we must reiterate that only strictly equilibrium properties have been here considered. Some of our results can be extricated from a previous paper on the complexified semiclassical approximation of quantum work and its employment in the Jarzynski equality [12]. But that was fundamentally a dynamical context, even if it may be considered in an adiabatic, quasi-statical limit. So it is important to gain a full clear view of the rich underlying pure statics. It should be pointed out that the present approximations are insensitive to any small effect of tunnelling under saddle points on steady states, if the Hamiltonian has more than one minimum.

Digging deeper, one may even question the central assumption that the thermal equilibrium of the system can be independent of the (in most cases) uncontrollable environment and their coupling, when viewed in a full quantum scenario. After all, the system Hamiltonian does not in general commute with the total Hamiltonian, which includes the system, the environment and their coupling, so one is implicitly assuming the limit of weak coupling. Indeed, the damping strength, characteristic of dissipative quantum evolution, will appear in the equilibrium state. In the partition function, this dependence on the damping strength is to be expected because it reflects the broadening of discrete eigenstates [4,37].

Notwithstanding the complexity of the general features of quantum equilibrium and the processes by which it is attained, it is of fundamental importance to be able to deal with thermal quantum systems on their own, described in their simplest form by the canonical density operator, that is, the quantum Gibbs ensemble. The thermal Wigner function presents this in a very convenient form, permitting the evaluation of the partition function and thermal averages as *classical* phase space integrals. The semiclassical approximation to the thermal Wigner function presented here bridges its extreme limits, while leading to simple quantum corrections to the classical high temperature limit. We have shown that attempting further saddle point approximations would discard most of the information contained in the full semiclassical theory. On the other hand, it is revealed that full content is preserved by a mere shift of the integration variable of a thermal average, which has the offshoot of dispensing with laborious searches for trajectories that are indirectly defined. No restriction to systems that satisfy the ordinary second order Schrödinger equation impinges on the present semiclassical approximation for the density operators of the canonical ensemble.

CRediT authorship contribution statement

Alfredo M. Ozorio de Almeida: Concept, Design, Analysis, Writing, or revision of the manuscript. **Gert-Ludwig Ingold:** Concept, Design, Analysis, Writing, or revision of the manuscript. **Olivier Brodier:** Concept, Design, Analysis, Writing, or revision of the manuscript.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Thermodynamic relations

The SC expectation of a smooth function of the Hamiltonian is a special case of (7.1), that is,

$$\langle F(\hat{H})\rangle_\beta \approx \frac{1}{Z_\beta}\int \mathrm{d}\mathbf{X}\ \left|\det\frac{\partial\mathbf{x}}{\partial\mathbf{X}}\right|^{1/2}\exp\ \ \frac{1}{\hbar}(S^i_{\hbar\beta}(\mathbf{x}(\mathbf{X})))\quad F(H(\mathbf{x})), \tag{A.1}$$

or equivalently the SC approximation to the thermal Wigner function is inserted directly in (1.6) to provide a macroscopic property of the system in complete thermal equilibrium with

its environment. In the case of the exact thermal average of the Hamiltonian itself the relation

$$\langle \hat{H} \rangle_\beta = -\frac{1}{Z_\beta}\frac{dZ_\beta}{d\beta} \tag{A.2}$$

is widely employed, even though there is an implicit assumption of an evolution of the temperature through the derivative, just as with the Jarzynski equality discussed in Section 8. Then, the strength of the coupling to the environment becomes relevant and indeed, one should restrict (A.2) to the limit of weak coupling [38]. In any case it is easily seen to hold formally, whereas it is more problematic within the full SC approximation.

Even though (A.2) is readily verified for a quadratic Hamiltonian (as it should, since here SC is exact), there are two major difficulties for general Hamiltonians. The first is that the amplitude of the Wigner function depends on β, not just its action. The amplitude cannot be taken out of the integral, since it also depends on $\mathbf{x}$, so that, on taking the derivative within the integral, there is a second term beyond the derivative of the exponential. The second problem is that, in taking the derivative of the exponent $S^r_{\hbar\beta}(\mathbf{x}(\mathbf{X}))$ itself, one obtains $H(\mathbf{X})$ instead of $H(\mathbf{x})$, together with the derivative of the integral in (6.9), which depends nonlinearly on β. Thus, the approximate satisfaction of the relation (A.2) depends on the counterbalancing of several terms and the direct evaluation of (A.1) should be preferred to the RHS of (A.2).

Curiously, both approximations (3.21) and (3.23), which account for the lowest quantum correction to the non-normalized thermal Wigner function, accommodate a version of the relation (A.2). Indeed, separating the exponent in the former into its linear and nonlinear parts,

$$\mathrm{e}^{-\beta H}(\mathbf{x}) \approx \frac{\exp\left[-\beta_1 H(\mathbf{x})\right]}{1+(\hbar\beta_2\Omega_{\mathbf{x}}/2)^2/2} \times \exp\left[-\frac{(\hbar\beta_2\Omega_{\mathbf{x}}/2)^3}{3}\,\frac{(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})\cdot\mathbf{H}_{\mathbf{x}}\,(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})}{\hbar\,\Omega_{\mathbf{x}}}\right]_{\beta_1=\beta_2=\beta}, \tag{A.3}$$

one obtains a *double-β partition function*

$$Z_{(\beta_1,\beta_2)} \equiv \int d\mathbf{x}\,\frac{\exp\left[-\beta_1 H(\mathbf{x})\right]}{1+(\hbar\beta_2\Omega_{\mathbf{x}}/2)^2/2} \times \exp\left[-\frac{(\hbar\beta_2\Omega_{\mathbf{x}}/2)^3}{3}\,\frac{(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})\cdot\mathbf{H}_{\mathbf{x}}\,(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}})}{\hbar\,\Omega_{\mathbf{x}}}\right] \tag{A.4}$$

and thus a lopsided version of (A.2):

$$\langle \hat{H} \rangle_\beta \approx -\frac{d\log Z_{(\beta_1,\beta_2)}}{d\beta_1}_{\beta_1=\beta_2=\beta}. \tag{A.5}$$

This same equality results from the isolation of the linear part of the exponent in the metaplectic Wigner function, with the alternative definition of a double-β partition function as

$$Z_{(\beta_1,\beta_2)} \equiv \int d\mathbf{x}\exp[-\beta_1 H(\mathbf{x})]\ \exp[\beta_2 H(\mathbf{x}-\boldsymbol{\gamma}_{\mathbf{x}}|\mathbf{H}_{\mathbf{x}})]\ \mathrm{e}^{-\beta_2 H}(\mathbf{x}-\gamma_{\mathbf{x}}|\mathbf{H}_{\mathbf{x}}). \tag{A.6}$$

Either of these definitions of a double-β partition function will again introduce a first quantum correction to further thermodynamic relations. The definition of the heat capacity again implies a dynamic (even if quasi-static) process of feeding in heat and for finite coupling to the environment its definition is no longer unique [38]. However, the assumption of weak coupling to the environment allows to relate the heat capacity to the second derivative of the partition function,

$$C \equiv \frac{d\langle\hat{H}\rangle_\beta}{dT} = \frac{-1}{k_B T^2}\frac{d\langle\hat{H}\rangle_\beta}{d\beta}$$

$$= \frac{1}{k_B T^2}\left[\left(\frac{1}{Z_\beta}\frac{dZ_\beta}{d\beta}\right)^2 - \frac{1}{Z_\beta}\frac{d^2 Z_\beta}{d\beta^2}\right]$$

$$= \frac{1}{k_B T^2}\left[\langle\hat{H}^2\rangle_\beta - \langle\hat{H}\rangle_\beta^2\right]. \tag{A.7}$$

The SC quantum correction at high temperatures is obtained as

$$C \approx \frac{1}{k_B T^2}\left[\left(\frac{1}{Z_{(\beta_1,\beta_2)}}\frac{dZ_{(\beta_1,\beta_2)}}{d\beta_1}\right)^2 - \frac{1}{Z_{(\beta_1,\beta_2)}}\frac{d^2 Z_{(\beta_1,\beta_2)}}{d\beta_1^2}\right]_{\beta_1=\beta_2=\beta}. \tag{A.8}$$

Again, at lower temperatures where one needs a full SC approximation for the thermal Wigner function, the relation for the specific heat is not transparently reproduced. Nevertheless, the variance of the energy, given by the final equality in (A.7), is easily obtainable through the general formula for expectations (7.1), whilst recalling that the Weyl representation $H^2(\mathbf{x})$ of $\hat{H}^2$ only equals the classical function $(H(\mathbf{x}))^2$, within a correction of order $\hbar$.

Appendix B. Comparing the semiclassical Wigner function with the exact one

B.1. Expression of the Wigner function for a normal form Hamiltonian

To evaluate the prefactor of the Weyl symbol of $\exp(-\beta\widehat{H})$, with $\widehat{H} = F(\frac{\mathbf{x}^2}{2})$, we use the expressions (4.5) and (5.8), leading to

$$e^{-\beta H}(\mathbf{x}(\mathbf{X})) \simeq \frac{e^{\frac{i}{\theta}\,\theta F'\left(\frac{\mathbf{x}^2}{2}\right) - \sinh\left(\theta F'\left(\frac{\mathbf{x}^2}{2}\right)\right)\left(\frac{\mathbf{x}^2}{2}-\frac{\theta}{\hbar}F\left(\frac{\mathbf{x}^2}{2}\right)\right)}}{\sqrt{\left|\det\left(\frac{\partial\mathbf{x}}{\partial\mathbf{X}}\right)\right|}}, \tag{B.1}$$

where $\mathbf{X}$ is the starting point for the pair of arcs evolving forward and backwards in time, and $\mathbf{x}$ is the middle of the chord joining the tips of that arc. In order to evaluate the above prefactor, we take the imaginary time version of the identity (4.3),

$$\mathbf{x} = \cosh\left(\frac{\theta}{2}F'\left(\frac{\mathbf{X}^2}{2}\right)\right)\mathbf{X}, \tag{B.2}$$

and we take its derivative with respect to $\mathbf{X} = (P, Q)$. We obtain

$$\frac{\partial\mathbf{x}}{\partial\mathbf{X}} = \cosh\left(\frac{\theta}{2}F'\left(\frac{\mathbf{X}^2}{2}\right)\right)\mathbf{I} + \frac{\theta}{2}F''\left(\frac{\mathbf{X}^2}{2}\right)\sinh\left(\frac{\theta}{2}F'\left(\frac{\mathbf{X}^2}{2}\right)\right)\mathbf{X}\mathbf{X}^\top, \tag{B.3}$$

which is of the form

$$\frac{\partial\mathbf{x}}{\partial\mathbf{X}} = \begin{matrix} C+SP^2 & SPQ \\ SQP & C+SQ^2 \end{matrix}, \tag{B.4}$$

and whose determinant is therefore

$$det\,\frac{\partial\mathbf{x}}{\partial\mathbf{X}} = C^2 + CS(P^2+Q^2), \tag{B.5}$$

so we have

$$det\,\frac{\partial\mathbf{x}}{\partial\mathbf{X}} = N\left(\frac{\mathbf{X}^2}{2}\right) \tag{B.6}$$

with

$$N(R) = \cosh^2\left(\frac{\theta F'(R)}{2}\right) + \theta R F''(R)\cosh\left(\frac{\theta F'(R)}{2}\right)\sinh\left(\frac{\theta F'(R)}{2}\right), \tag{B.7}$$

and the expression of $\exp(-\beta\widehat{H})$ follows

$$e^{-\beta H}(\mathbf{x}(\mathbf{X})) \simeq \frac{e^{\frac{1}{\hbar}\theta F'\frac{\mathbf{X}^2}{2} - \sinh\theta F'\frac{\mathbf{X}^2}{2}\left(\frac{\mathbf{X}^2}{2} - \frac{\theta}{\hbar}F\frac{\mathbf{X}^2}{2}\right)}}{\cosh\left[\frac{\theta}{2}F'\frac{\mathbf{X}^2}{2}\right]\sqrt{1+\theta\frac{\mathbf{X}^2}{2}F''\frac{\mathbf{X}^2}{2}\tanh\left[\frac{\theta}{2}F'\frac{\mathbf{X}^2}{2}\right]}}. \tag{B.8}$$

On the other hand, we can have an expression for the exact Weyl symbol by using its decomposition in the basis of the harmonic oscillator $\{|n\rangle\}$, that is

$$e^{-\beta\widehat{H}} = \sum_{n=0}^{\infty} e^{-\beta F\hbar\left(n+\frac{1}{2}\right)}|n\rangle\langle n| \tag{B.9}$$

with

$$\frac{\widehat{\mathbf{x}}^2}{2}|n\rangle = \hbar\left(n+\frac{1}{2}\right)|n\rangle, \tag{B.10}$$

then, knowing that the Weyl symbol of $|n\rangle\langle n|$ is given by (2.2), we have

$$e^{-\beta H}(\mathbf{x}) = \sum_{n=0}^{\infty} e^{-\frac{\theta}{\hbar}F\hbar\left(n+\frac{1}{2}\right)}\frac{(-1)^n}{\pi\hbar}e^{-\frac{\mathbf{x}^2}{\hbar}}L_n\left(\frac{2\mathbf{x}^2}{\hbar}\right). \tag{B.11}$$

Now, to compare (B.8) with (B.11), we need to put the latter with the same variable $\mathbf{X}$, which requires to use expression (B.2),

$$e^{-\beta H}(\mathbf{x}(\mathbf{X})) = \sum_{n=0}^{\infty}\frac{(-1)^n}{\pi\hbar}e^{-\frac{\theta}{\hbar}F\hbar\left(n+\frac{1}{2}\right) - \frac{1}{\hbar}\mathbf{x}^2\cosh\frac{\theta}{2}F'\frac{\mathbf{X}^2}{2}}{}^{2} \times L_n\left(\frac{2}{\hbar}\mathbf{X}^2\cosh\frac{\theta}{2}F'\frac{\mathbf{X}^2}{2}\right)^2\Bigg). \tag{B.12}$$

B.2. Partition function

The partition function in the Weyl–Wigner representation is given by

$$Tr\left(e^{-\beta\widehat{H}}\right) = \frac{1}{2\pi\hbar}\int e^{-\beta H}(\mathbf{x})\, d^2\mathbf{x}. \tag{B.13}$$

To benefit from the simple expression of the action used in this article, we change the variable from the midpoint $\mathbf{x}$ of the chord to the starting point of the arc $\mathbf{X}$, related by (B.2), and obtain

$$Tr\left(e^{-\beta\widehat{H}}\right) = \frac{1}{2\pi\hbar}\int e^{-\beta H}(\mathbf{x}(\mathbf{X}))\left|\det\frac{\partial\mathbf{x}}{\partial\mathbf{X}}\right| d^2\mathbf{X}. \tag{B.14}$$

Then, noticing that the Jacobian of this change of variable is the square of the inverse of the prefactor which appears in (B.1), the semiclassical expression for $e^{-\beta H}(\mathbf{x}(\mathbf{X}))$, we get $Tr\left(e^{-\beta\widehat{H}}\right) \simeq Z_{sc}$ with

$$Z_{sc} = \frac{1}{2\pi\hbar}\int e^{\frac{1}{\hbar}\sigma_\theta\frac{\mathbf{X}^2}{2}}\sqrt{\left|\det\frac{\partial\mathbf{x}}{\partial\mathbf{X}}\right|}\, d^2\mathbf{X}, \tag{B.15}$$

with

$$\sigma_\theta\left(\frac{\mathbf{X}^2}{2}\right) = \theta F'\frac{\mathbf{X}^2}{2} - \sinh\theta F'\frac{\mathbf{X}^2}{2}\left(\frac{\mathbf{X}^2}{2} - \theta F\frac{\mathbf{X}^2}{2}\right). \tag{B.16}$$

Then, according to (B.6),

$$Z_{sc} = \frac{1}{2\pi\hbar}\int e^{\frac{1}{\hbar}\sigma_\theta\frac{\mathbf{X}^2}{2}}\sqrt{N\left(\frac{\mathbf{X}^2}{2}\right)}\, d^2\mathbf{X}. \tag{B.17}$$

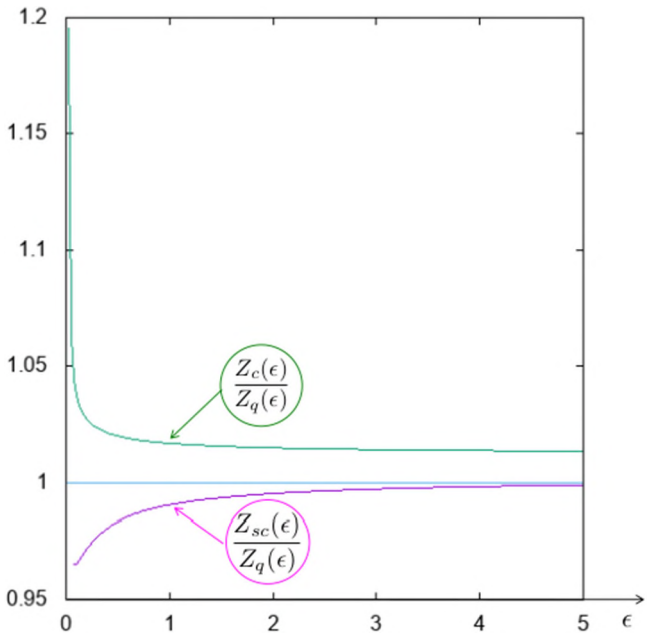

Fig. B.1. Ratio Z_{sc}/Z_q as a function of ϵ, for $\hbar = 0.2$ and $\omega = 0.5$. The semiclassical partition function Z_{sc} deviates from the exact quantum one, Z_q, in the homogeneous limit $\epsilon \to 0$. The ratio of the classical partition function Z_c to the latter is also shown.

Applying the change of variables, $\mathbf{X} = \sqrt{2u}\cos\phi, \sqrt{2u}\sin\phi$, so that $u = \mathbf{X}^2/2$, one has $d^2\mathbf{X} = du d\phi$, and, integrating over ϕ, we are left with a single integral

$$Z_{sc} = \frac{1}{\hbar}\int_0^{\infty} e^{\frac{1}{\hbar}\sigma_\theta(u)}\sqrt{N(u)}\, du. \tag{B.18}$$

On the other hand, the exact partition function is given by

$$Z_q = \sum_{n=0}^{\infty} e^{-\beta F\hbar\left(n+\frac{1}{2}\right)} = \sum_{n=0}^{\infty} e^{-\frac{\theta}{\hbar}F\hbar\left(n+\frac{1}{2}\right)}. \tag{B.19}$$

As a comparison, the classical partition function is

$$Z_c = \int_0^{\infty} e^{-\frac{\theta}{\hbar}F(y)}\, dy. \tag{B.20}$$

Notice that Z_{sc} contains the integrand of Z_c, but multiplied by a function, that is

$$Z_{sc} = \frac{1}{\hbar}\int_0^{\infty} e^{-\frac{\theta}{\hbar}F(u)}e^{\frac{1}{\hbar}\Delta_\theta(u)}\sqrt{N(u)}\, du, \tag{B.21}$$

with

$$\Delta_\theta(u) = u\left[\theta F'(u) - \sinh\left(\theta F'(u)\right)\right]. \tag{B.22}$$

B.3. Some example

Let us take, as an example, a general nonhomogeneous Kerr oscillator, that is

$$H(\mathbf{x}) = \omega\frac{\mathbf{x}^2}{2} + \frac{\omega^2}{}\left(\frac{\mathbf{x}^2}{2}\right)^2. \tag{B.23}$$

This corresponds to

$$F(u) = \omega u + \frac{\omega^2}{}u^2 \quad F'(u) = \omega + 2\frac{\omega^2}{}u \quad F''(u) = 2\frac{\omega^2}{}, \tag{B.24}$$

so the semiclassical partition function writes

$$Z_{sc} = \int_0^\infty e^{\frac{u}{\hbar}\left[\frac{\theta\omega^2 u}{2}-\sinh\left(\frac{\theta\omega}{2}+\frac{\theta\omega^2 u}{2}\right)\cosh\left(\frac{\theta\omega}{2}+\frac{\theta\omega^2 u}{2}\right)\right]} \times \sqrt{1+\frac{2\theta\omega^2 u\,\tanh\left(\frac{\theta\omega}{2}+\frac{\theta\omega^2 u}{2}\right)}{\hbar}}\,du. \tag{B.25}$$

Fig. B.1 compares the semiclassical, the quantum and the classical partition function as a function of ϵ. Obviously the semiclassical approximation loses accuracy for the purely Kerr Hamiltonian.

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