Weyl–Wigner representation of canonical equilibrium states

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Abstract

The Weyl–Wigner representations for canonical thermal equilibrium quantum states are obtained for the whole class of quadratic Hamiltonians through a Wick rotation of the Weyl–Wigner symbols of Heisenberg and metaplectic operators. The behavior of classical structures inherently associated to these unitaries is described under the Wick mapping, unveiling that a thermal equilibrium state is fully determined by a complex symplectic matrix, which sets all of its thermodynamical properties. The four categories of Hamiltonian dynamics (parabolic, elliptic, hyperbolic and loxodromic) are analyzed. Semiclassical and high temperature approximations are derived and compared to the classical and/or quadratic behavior.

Keywords: quadratic Hamiltonians, Weyl–Wigner formalism, Wick rotation, thermal states, canonical equilibrium

((Some figures may appear in colour only in the online journal)

Following the statistical physics postulates [1], the state of a system in equilibrium with a canonical thermal reservoir is described by the density operator

\[ \hat{\rho}_T = \frac{e^{-\beta \hat{H}}}{Z_\beta}, \quad Z_\beta := \text{Tr} e^{-\beta \hat{H}}, \]  

(1)

where \( \beta := (k_B T)^{-1} \in \mathbb{R} \) is the ‘inverse temperature’, \( k_B \) is the Boltzmann constant and \( \hat{H} \) is the Hamiltonian of the system. The partition function (PF) \( Z_\beta \) provides the normalization of the state and is a central object of the theory, since it is the first step toward the derivation of thermodynamical function and potentials [1].

The evolution of a (time independent) quantum system is performed by the unitary operator

\[ \hat{U}_t := e^{-i\hat{H}t/\hbar}, \]  

(2)

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which can be related to the thermal state in (1) through
\[ t \mapsto -i\hbar\beta. \] (3)

This simple holomorphic mapping, known as Wick rotation [2], is particularly useful and constitutes basic tool for quantum field theory, see for instance [3, 4], where propagators (path-integrations in Minkowski space) are mapped into Euclidean path integrals. Surprisingly enough, hardly one will find this subject in statistical mechanics textbooks [5], and only two examples, the free particle and the harmonic oscillator, are presented in the standard quantum mechanics literature [6].

The mentioned examples are embraced by the wider category of the systems described by quadratic Hamiltonians (QH), which constitute the basic building blocks for the study of conservative dynamical systems in classical and in quantum mechanics [7, 8]. For this category, a group theoretical approach elegantly combines classical and quantum mechanics over a phase-space background supplied by the Weyl–Wigner–Moyal description of quantum mechanics [9–12].

For generic quantum dynamics, semiclassical approximations are useful methods to describe the system behavior when the constant \( \hbar \) is very small when compared to a characteristic action, which roughly constitutes the limit \( \hbar \to 0 \) [7, 8]. In this limit, inherent classical structures emerge, e.g., the famous WKB method shows that the phase of the wave function is governed by a classical Hamilton–Jacobi equation [7, 8]. QHs provides, by one side, the best known examples of application for semiclassical methods in what concerns the quantum–classical correspondence [7, 8]. By another side, some of the semiclassical techniques are exact for such kind of Hamiltonians, for instance, the Moyal bracket collapses into the classical Poisson bracket [13], while for any other non-trivial Hamiltonian, it constitutes an expansion in powers of \( \hbar \).

QHs are the commonly realizable operations in optics laboratories for the manipulation of the continuous degrees of freedom (quadratures) of electromagnetic field [14]. Nowadays, these powerful techniques are also devoted to encoding, manipulate, transport, and store information by quantum protocols associated to continuous degrees of freedom states [15]. Thermal states of the electromagnetic field occupies a privileged position at this scenario, due to a lack of a Weyl–Wigner description (or any other equivalent) for all thermal states, distinct theoretical methods were developed just to determine ensemble averages at non-zero temperatures [16] and the Wigner function itself for some QH thermal states [17].

In the scope of open quantum system dynamics, the Markovian interaction of continuous-variable quantum system with an external and uncontrollable environment can lead the system to a steady-state [18]. Theoretically, thermal equilibrium states (1) associated to QHs can be generated by an appropriate environmental interaction [19]. The robustness of the steady-state, since it does not depend on the initial state, but only on the environment, is a valuable tool for state engineering, stabilization and design, as detailed in [19] and the references therein.

In this work, the Wigner–Weyl symbols (and thus, the Wigner and the characteristic function) of canonical thermal equilibrium states will be determined for the whole class of systems described by QHs with a generic number of degrees of freedom. The derivation is performed applying a Wick rotation to the Weyl–Wigner symbols associated to groups of unitary operators, named Heisenberg and metaplectic. These operators are quantum representations of classical translations and (real) symplectic transformations. The generality of the results obtained for any QH is due to the duality between the Wigner and the Weyl representations, where an unavoidable divergence of one is compensated by the well behavior of the other.

The set of thermal states is shown to be completely described by a complex symplectic group raised by a Wick rotation of the classical phase-space. Interesting enough, the categorization of
the four types of classical symplectic dynamics (parabolic, elliptic, hyperbolic and loxodromic) is extended to the thermal states and examples are given. The elliptic case corresponds to the class of positive-definite QH, which includes the harmonic oscillator system; it is the only case where both Wigner–Weyl symbols are Gaussians and has been extensively studied in the literature, see for instance [20]. The inherent covariance of symbols under linear canonical transformations when applied to thermal states does not change thermodynamical properties of each category. Limits on temperature and on \( \hbar \) show connections between the quantum and classical thermal states.

This work is organized as follows. Section 1 begins with the Weyl–Wigner formalism description and finishes with the Wick rotation of the unitary symbols. The structure of the classical canonical transformations and their Wick rotated version are placed in section 2. The unitary subgroups related to the classical canonical transformations are described in section 3, while the symbols for the thermal equilibrium states and their properties are calculated and determined in section 4. Approximations for non-QHs are in section 5. In section 6, several examples of thermal states generated by QHs are given and its properties analyzed according to the four categories of symplectic matrices. Finally, the conclusions and perspectives are presented in section 7.

1. Weyl–Wigner formalism

Consider a quantum systems described by \( n \) continuous bosonic degrees of freedom. The generalized coordinates \( \bar{q} := (q_1, \ldots, q_n) \) together with the canonical conjugated momenta \( \bar{p} := (p_1, \ldots, p_n) \) are written collectively as a \( 2n \)-column-vector: \( \bar{x} := (\bar{q}, \bar{p}) \).

In this notation, the canonical commutation relation (CCR) is written compactly as

\[
\hat{J} := \begin{pmatrix} I_n & 0_n \\ -0_n & I_n \end{pmatrix} = -\hat{J}^\top = -\hat{J}^{-1}.
\]

(4)

The Weyl translation (or the Heisenberg operator) is an unitary operator defined as [10]

\[
\hat{T}_\xi := \exp \left[ -\frac{i}{\hbar} \hat{x} \wedge \xi \right], \quad \hat{x} \wedge \xi := \hat{J} \cdot \xi,
\]

(5)

where the column vector \( \xi := (\xi_1, \ldots, \xi_{2n}) \in \mathbb{R}^{2n} \) sets the direction of a translation of the operator \( \hat{x} \), i.e., \( \hat{T}_\xi \hat{x} \hat{T}_\xi^{-1} = \hat{x} + \xi \). The parity operator [6] will be denoted \( \hat{R}_0 \) and its action is described by \( \hat{T}_{\hat{R}_0} \hat{x} \hat{R}_0 = -\hat{x} \). It is an involutory operator, since \( \hat{R}_0^2 = 1 \), and thus \( \hat{R}_0 = \hat{R}_0^{-1} = \hat{R}_0^{-1} \). The reflection operator is defined as [10]

\[
\hat{R}_s := \hat{T}_s \hat{R}_0 \hat{T}_s^\dagger = \hat{R}_s^\dagger = \hat{R}_s^{-1},
\]

(6)

where \( x := (q_1, \ldots, p_n) \) is a column vector indicating the reflection point, i.e., \( \hat{R}_s \hat{x} \hat{R}_s = -\hat{x} + 2x_1 \).

Both sets of translations and of reflections constitute a basis for the vector space of the operators acting on the Hilbert space of a continuous variable quantum system, i.e., an arbitrary operator \( \hat{A} \) can be uniquely expanded as

\[
\hat{A} = \int \frac{d^{2n}\xi}{(2\pi\hbar)^n} \hat{A}(\xi) \hat{T}_\xi = \int \frac{d^{2n}x}{(\pi\hbar)^n} A(x) \hat{R}_s,
\]

(7)

where the column vector \( \xi \) is defined as [10]
which are, respectively, the Weyl and the Wigner representations of $\hat{A}$ [10]. The coefficients $\tilde{A}(\xi)$ and $A(x)$ are, respectively, defined through the inner products

$$\tilde{A}(\xi) = \text{Tr}(\hat{A}\hat{T}^+_\xi), \quad A(x) = 2^n \text{Tr}(\hat{A}\hat{R}_x),$$

by virtue of [10]

$$\text{Tr}(\hat{T}_\xi\hat{T}^+_\xi) = 2^{2n} \text{Tr}(\hat{R}_\xi\hat{R}_\xi) = (2\pi\hbar)^n \delta^{2n}(\xi - \xi').$$

It is also important to mention that

$$\text{Tr}(\hat{T}_\xi) = (2\pi\hbar)^n \delta^{2n}(\xi), \quad \text{Tr}(\hat{R}_\xi) = 1/2^n.$$

The coefficients in (8) are known, respectively, as the Weyl and Wigner symbols of the operator $\hat{A}$. The change of basis (6) relates these symbols through a symplectic Fourier transform, viz,

$$\tilde{A}(\xi) = \int \frac{d^2x}{(2\pi\hbar)^n} A(x)e^{i\hbar x \cdot \xi}.$$

In particular, the Wigner function $W(x)$ of a quantum state is (a normalized version of) the Wigner symbol associated with the corresponding density operator $\hat{\rho}$ [10, 21], that is,

$$W(x) := \frac{1}{(\pi\hbar)^n} \text{Tr}[\hat{\rho}\hat{R}_x].$$

Its symplectic Fourier transform is the characteristic function (the Weyl symbol) of $\hat{\rho}$ [10]:

$$\chi(\xi) = \int \frac{d^2x}{(2\pi\hbar)^n} W(x)e^{i\hbar x \cdot \xi} = \frac{1}{(2\pi\hbar)^n} \text{Tr}[\hat{\rho}\hat{T}_\xi].$$

1.1. Equilibrium states, unitary operators and Wick rotation

The Weyl–Wigner symbols for the canonical equilibrium state in (1) are determined, respectively, by (12) and (13). However, it is interesting to describe the symbols for the operator $\exp(-\beta \hat{H})$ and the PF as a functional of these symbols. Thus, considering the expansions in (7), the symbols (8) for the thermal operator are

$$\tilde{E}_\beta(\xi) := \text{Tr}(e^{-\beta \hat{H}}\hat{T}^+_\xi), \quad E_\beta(x) := 2^n \text{Tr}(e^{-\beta \hat{H}}\hat{R}_x).$$

Complex conjugating and taking into account that the thermal operator is Hermitian, above symbols (actually the symbols of any Hermitian operator) are such that

$$\tilde{E}_\beta(\xi) = [\tilde{E}_\beta(-\xi)]^*, \quad E_\beta(x) = [E_\beta(x)]^*.$$

Taking the trace of (7) and using (10), the expression for the PF of the thermal state as functionals of the symbols becomes

$$Z_\beta := \text{Tr} e^{-\beta \hat{H}} = \tilde{E}_\beta(0) = \frac{1}{(2\pi\hbar)^n} \int d^2x E_\beta(x),$$

where the second equality is a manifestation of the independence of the trace on a specific basis.
Joining (14) and (16), the characteristic and Wigner functions of the thermal state (1) are
\[ \chi(\xi) = \frac{\tilde{E}_\beta(\xi)}{(2\pi\hbar)^n E_\beta(0)}, \quad W(x) = \frac{E_\beta(x)}{\int d^2x E_\beta(x)}, \]
(17)
as they should be from the definitions (12) and (13).

The expansions in (7) for the unitary operator in (2) are
\[ \tilde{U}_t(\xi) = \text{Tr}(\hat{U}_t \hat{T}_\xi^\dagger), \quad U_t(x) = 2^n \text{Tr}(\hat{U}_t \hat{R}_x), \]
(18)
and taking into account that \( \hat{U}_t^\dagger = \hat{U}_{-t} \), above symbols are, respectively, such that
\[ \tilde{U}_{-t}(\xi) = [\tilde{U}_t(-\xi)]^*, \quad U_{-t}(x) = [U_t(x)]^*. \]
(19)

Since any operator can be expressed as a linear combination of translations or reflections, the Wick rotation (3) is readily applicable to the level of the coefficients of the expansion, i.e., the Weyl–Wigner symbols. However, to take into account the nature of the operators at the symbols level, which are explicitly manifested in (15) and (19), it is preferable to express the Wick mapping as
\[ \tilde{E}_\beta(\xi) = \frac{1}{2} U_{-i\hbar\beta}(\xi) + \frac{1}{2} [U_{-i\hbar\beta}(-\xi)]^*, \quad E_\beta(x) = \text{Re} \left[ U_{-i\hbar\beta}(x) \right]. \]
(20)

For the purposes of this work, it is sufficient to consider \( \tilde{E}_\beta(\xi) = \tilde{U}_{-i\hbar\beta}(\xi) \) and \( E_\beta(x) = U_{-i\hbar\beta}(x) \) instead of above equations, however equation (20) are suitable for generalizations, for instance, in the case of time-dependent Hamiltonians. The inverse mapping is
\[ \tilde{U}_t(\xi) = \tilde{E}_{it/\hbar}(\xi), \quad U_t(x) = E_{it/\hbar}(x). \]

Even though the problem seems to be solved by equation (20), the obtainment of \( U_t(x) \) or \( \tilde{U}_t(\xi) \) analytically is rare and restricted to few cases. In general, one considers (semiclassical) approximations valid for limited time intervals [10, 11]. Even for QHs, the obtainment of the propagator (unitary operator expanded in a certain basis) is not a trivial question. Remember that a closed expression for the propagator of the Harmonic oscillator in quantum mechanics textbooks relies on the celebrated, as well as intricate, Mehler formula for a sum of products of Hermite polynomials [6].

Fortunately, the dynamics of quantum systems evolves by a generic QH nowadays is elegantly developed though a theoretical group representation approach based on classical dynamics.

2. Symplectic evolution

This section reviews some facts about classical QHs and also includes, at the end, a discussion about their Wick rotated version, both of which will be necessary for the constructions of the Wigner–Weyl symbols.

The simplest non-trivial evolution of a mechanical system is described by the linear Hamiltonian
\[ H_1 = x \wedge \zeta + H_0, \]
(21)
where $\zeta \in \mathbb{R}^{2n}$ is a constant column vector and $H_0 \in \mathbb{R}$ is a constant. Under $H_1(x)$, an initial condition in phase space $x_0 \in \mathbb{R}^{2n}$ evolves to $\varphi_1(x_0, t) = x_0 + \zeta t$. The Hamiltonians (21) constitute the Heisenberg Lie algebra $h(2n)$ under the Poisson bracket operation.

A ‘new’ Hamiltonian $H'_1 = x \wedge \zeta' + H'_0$ generates the flux $\varphi'_1(x_0, t) = x_0 + \zeta' t$; since $\varphi'_1 \circ \varphi_1(x_0, t) = x_0 + (\zeta + \zeta') t$, the flux of these Hamiltonian are members of an additive Abelian group, sometimes also called the Heisenberg group of translations $H(2n)$, generated by vectors $J \otimes \zeta \in \mathbb{R}^{2n}$.

Consider now the classical QH

$$H_2 := \frac{1}{2} x \cdot \mathbf{H} x,$$

where $\mathbf{H} = \mathbf{H}^\top \in \text{Mat}(2n, \mathbb{R})$ is the Hessian matrix. The set of these Hamiltonians constitutes a Lie algebra (under the Poisson bracket) dubbed metaplectic algebra $\mathfrak{mp}(2n)$ [11, 12]. The phase-space flux of (22) is $\varphi_2(x_0, t) = \mathbf{S}_t x_0$, where

$$\mathbf{S}_t := \exp[J\mathbf{H}t]$$

is an element of the real symplectic group $\text{Sp}(2n, \mathbb{R}) := \{ \mathbf{M} \in \text{Mat}(2n, \mathbb{R}) | \mathbf{M}^\top \mathbf{J} \mathbf{M} = \mathbf{J} \}$ for $\mathbf{J}$ in (4).

Not all matrices $\mathbf{M} \in \text{Sp}(2n, \mathbb{R})$ can be written as (23), while matrices of the form (23) constitutes an uniparametric subgroup of $\text{Sp}(2n, \mathbb{R})$ for a given generator (also called Hamiltonian matrix) $\mathbf{J} \mathbf{H} \in \text{sp}(2n)$, where $\text{sp}(2n)$ is the symplectic Lie algebra. Any symplectic matrix $\mathbf{M} \in \text{Sp}(2n, \mathbb{R})$ is such that $\det \mathbf{M} = 1$, since $\mathbf{J} = \mathbf{M}^\top \mathbf{J} \mathbf{M}$ implies [12]

$$\text{Pf}(\mathbf{J}) = \text{Pf}(\mathbf{M}^\top \mathbf{J} \mathbf{M}) = (\det \mathbf{M})\text{Pf}(\mathbf{J}),$$

where the second equality is a property of the Pfaffian [22].

The Hamiltonian nature of the generators $\mathbf{J} \mathbf{H} \in \text{sp}(2n)$ imposes strong constrains to the symplectic dynamics. The characteristic polynomial

$$P(\lambda) := \det(\mathbf{J} \mathbf{H} - \lambda I_{2n}) = \det(H \mathbf{J}^\top - \lambda I_{2n})$$

$$= \det(J^\top \mathbf{H} - \lambda I_{2n}) = P(-\lambda),$$

as shown, is an even function of $\lambda$. Furthermore, a complex eigenvalue always appears together with its complex conjugate, since $\det(\mathbf{J} \mathbf{H}) \in \mathbb{R}$. These constrains show that the eigenvalues of a Hamiltonian matrix $\mathbf{J} \mathbf{H}$ must fall into four cases [23]:

(P) Parabolic: a pair of null eigenvalues;
(H) Hyperbolic: a pair $(k, -k)$ for $k \in \mathbb{R}$;
(E) Elliptic: a pair $(i\omega, -i\omega)$ for $\omega \in \mathbb{R}$;
(L) Loxodromic: a quartet $(\gamma, -\gamma, \gamma^*, -\gamma^*)$ for $\gamma \in \mathbb{C}$.

A Jordan decomposition can be employed through the construction of a transition matrix $\mathbf{Q} \in \text{Mat}(2n, \mathbb{R})$ such that $\mathbf{QJHQ}^{-1} = \mathbf{J}$, where $\mathbf{J}$ is the matrix composed by the Jordan blocks associated to the above eigenvalues. Consequently, the eigenvalues of $\mathbf{S}_t$ in (23) are exactly the exponential of the ones above. Actually, this classification holds for any $\mathbf{S} \in \text{Sp}(2n, \mathbb{R})$ [8, 23].

Note that the elements of $\mathfrak{mp}(2n)$ and of $\mathfrak{sp}(2n)$ are in an one-to-one correspondence, which is not true for $\mathfrak{sp}(2n)$ and $\mathfrak{Sp}(2n, \mathbb{R})$ since two distinct values of the parameter $t$ can give rise to the same symplectic matrix $\mathbf{S}_t$ in (23). This duplicity is controlled by a topological quantity
associated to $\text{Sp}(2n, \mathbb{R})$ dubbed Conley–Zehnder (CZ) index \[24\], which will be defined in the context of unitary operators, see section 3.2.

Finally, the most generic QH is

$$H_\alpha := H_1 + H_2 = \frac{1}{2} \mathbf{v} \cdot \mathbf{H} \mathbf{x} + \mathbf{x} \wedge \zeta + H_0,$$

which is a member of the inhomogeneous metaplectic Lie algebra denoted by $\text{Imp}(2n)$ and generates the flux

$$\varphi(x_0, t) = S_t x_0 + \int_0^t d\tau S_\tau \zeta, \quad S_t = \exp[JHt].$$

2.1. Wick rotation of classical dynamics

The action of the Wick rotation (3) on the classical flux is determined by the transformed Hamilton equations, viz, for a time independent Hamiltonian

$$\frac{dx}{dt} \rightarrow \frac{i}{\hbar} \frac{dx}{d\beta} = J \frac{\partial H}{\partial x} \implies \frac{dx}{d\beta} = -i\hbar J \frac{\partial H}{\partial x}. \quad (27)$$

On this account, the flux generated by the QH in (26) is

$$\varphi(x_0, \beta) = S_{-i\hbar \beta} x_0 - i\hbar \int_0^{-i\hbar \beta} d\tau S_\tau \zeta,$$

where the path of integration is along the imaginary axis and

$$S_{\beta} := S_{-i\hbar \beta} = \exp[-i\hbar \beta JH] = (S_{\beta}^*)^{-1}. \quad (28)$$

The Wick rotation, from (27), is a simple multiplication of the generators by a complex constant:

$$JH \mapsto -i\hbar JH, \quad J\zeta \mapsto -i\hbar J\zeta, \quad (29)$$

which does not change the corresponding Lie algebras $\mathfrak{h}(2n)$ and $\mathfrak{sp}(2n)$ themselves. The matrix $S_{\beta}$ belongs to the complex symplectic group $\text{Sp}(2n, \mathbb{C}) := \{ S \in \text{Mat}(2n, \mathbb{C}) | S^T J S = J \}$, since

$$J S_{\beta}^T J = J \exp[i\hbar \beta JH] J^T = \exp[i\hbar \beta JH] = S_{\beta}^{-1},$$

which is equivalent to the symplectic condition and, accordingly to (24), det $S_{\beta} = 1$. Additionally, $S_{\beta}$ satisfies

$$S_{\beta}^* = S_{\beta}^{-1}, \quad \text{Tr } S_{\beta} \in \mathbb{R}, \quad (30)$$

which are properties not shared by all matrices in $\text{Sp}(2n, \mathbb{C})$. It is thus convenient to define the Wick rotated version of the real symplectic group by

$$\text{WSp}(2n, \mathbb{C}) := \{ S \in \text{Sp}(2n, \mathbb{C}) | S^* = S^{-1} \} \subseteq \text{Sp}(2n, \mathbb{C}).$$

Due to (29), $\text{WSp}(2n, \mathbb{C})$ and $\text{Sp}(2n, \mathbb{R})$ share the same Lie algebra, viz, $\mathfrak{sp}(2n)$ and the Wick rotation does preserve the categorization into (P), (H), (E) and (L), since it is a constrain on the generators $JH \in \mathfrak{sp}(2n)$. However, the uniparametric subgroups of (23) and of (28) can not
belong always to the same category, due to the complex nature of the rotation: categories (P) and (L) are invariant, while categories (H) and (E) are interchanged. In short,

\[
t \mapsto -i \hbar \beta \Rightarrow \begin{cases} 
(P) \rightarrow (P); \\
(L) \rightarrow (L); \\
(H) \leftrightarrow (E).
\end{cases}
\]  

(31)

By the end, the structural difference between the relation of the symplectic groups, real and complex, with their respective uniparametricsubgroups should be highlighted, and relies on properties (30). As already mentioned, a generic symplectic matrix \( S \in \text{Sp}(2n, \mathbb{R}) \) has not the form in (23), however it is always decomposable as a product of matrices like the one in (23), of course, with different generators [12, 25]. In contrast, generic complex matrices in \( \text{Sp}(2n, \mathbb{C}) \) have complex trace, thus they cannot be written as a matrix in (28), neither can be decomposed as a product of such matrices.

3. Subgroups of unitary evolutions

Time-evolution operators of quantumsystems constitutes a subgroup of the unitary operators. This section describes the unitary representation of those subgroups presented previously on section 2. In addition, the group of translations and reflections will also be discussed, since it is necessary to perform calculations with the symbols in section 1.

3.1. Heisenberg group and reflections

Using the Zassenhaus (or BHC) formula [6] and the CCR, the composition of two Weyl operators in (5) is

\[
\hat{T}_\xi \hat{T}_{\xi'} = \exp \left[ \frac{i}{2\hbar} \xi' \wedge \xi'' \right] \hat{T}_{\xi' + \xi''};
\]  

(32)

thus the set of Weyl operators constitutes a continuous Lie group, which is a representation of the Heisenberg group \( H(2n) \) [9–12]. The quantization of the classical Hamiltonian (21) with \( H_0 = 0, H_1(x) = \hat{x} \wedge \zeta \), is the generator of an uniparametric subgroup of Weyl operators. Like its classical version, the set of these Hamiltonians constitutes the Lie algebra \( h(2n) \) under the commutator operation.

In contrast, a reflection, as parity, is not continuous and their set even constitutes a group, both of which are evident from the composition rule

\[
\hat{R}_x \hat{R}_x' = \exp \left[ -\frac{2i}{\hbar} x' \wedge x'' \right] \hat{T}_{2(x'-x')},
\]  

(33)

that can be derived from (6). However, following [10], the composition of a reflection and a translation,

\[
\hat{R}_x \hat{T}_\xi = \exp \left[ \frac{i}{\hbar} \xi \wedge x \right] \hat{R}_{-\frac{\xi}{2}},
\]  

(34)

is a reflection. The product rules (6), (33) and (34) show that the set \( \text{Oz}(2n) := H(2n) \cup \{\hat{R}_0\} \) is a (discrete) group of translations and reflections [10].
From the definitions in (8), using accordingly the compositions (33) or (34), and equation (9), the symbols of the elements in $Oz(2n)$ are
\[
\tilde{T}_\eta(\xi) = (2\pi\hbar)^n\delta^{2n}(\eta - \xi), \quad T_\eta(x) = e^{-\frac{i}{\hbar}X^*_\eta};
\]
\[
\tilde{R}_\eta(\xi) = e^{\frac{i}{\hbar}X^*_\eta}, \quad R_\eta(x) = (\pi\hbar)^n\delta^{2n}(x - \eta).
\]
(35)

### 3.2. Metaplectic group and Conley–Zehnder index

For $S \in \text{Sp}(2n, \mathbb{R})$, an unitary operator $\hat{M}_S$ such that
\[
\hat{M}_S^\dagger \hat{M}_S = S \hat{x}
\]
is called a metaplectic operator (MO) and is a member of the subgroup of the unitary operators called metaplectic group and denoted by $\text{Mp}(2n)$ [11, 12].

The symmetric quantization of (22),
\[
\hat{H}_2 = \frac{1}{2} \hat{x} \cdot \hat{H} \hat{x},
\]
is an element of the metaplectic Lie algebra $\mathfrak{mp}(2n)$, the same algebra of the classical Hamiltonians (22), but now under the commutator operation [11, 12]. Thus, an uniparametric subgroup of $\text{Mp}(2n)$ is constituted by
\[
\tilde{M}_S := \exp \left[ -\frac{it}{2\hbar} \hat{x} \cdot \hat{H} \hat{x} \right],
\]
(38)
where the subindex $S$ highlights the relation between the MO and the symplectic matrix (23). It is important to stress that not all operators defined through (36) are like the ones in (38).

As for the classical dynamics, for each element (37) in $\mathfrak{mp}(2n)$, which is in one-to-one correspondence with $\mathfrak{sp}(2n)$, there are two in $\text{Mp}(2n)$ and it is said that the metaplectic group is a double covering group of the symplectic one [12]. This will be clear from the analyses of the symbols related to the MOs.

The Weyl and Wigner symbols (8) of a generic MO are given [10, 12, 26], respectively, by
\[
\tilde{M}_S(\xi) = \exp \left[ -\frac{i}{\hbar} \xi \cdot J C^{-1}_S J_\xi \right] \sqrt{\det (S - I_{2n})},
\]
(39)
and
\[
M_S(x) = 2^n \exp \left[ -\frac{i}{\hbar} x \cdot C_S x \right] \sqrt{\det (S + I_{2n})},
\]
(40)
where $C_S \in \text{Mat}(2n, \mathbb{R})$ stands for the Cayley parametrization of $S \in \text{Sp}(2n, \mathbb{R})$ defined by
\[
C_S := -\sqrt{\frac{(S - I_{2n})}{(S + I_{2n})}} = C_S^\dagger = -C_{S^{-1}}.
\]
(41)

Accordingly with $S$, one or both of the above symbols may not be defined, which happens when $\pm 1 \in \text{Spec}(S)$, i.e., when $\det (S \pm I_{2n}) = 0$. These discontinuities are definitely not a property of the operator itself, it is an unavoidable feature of the expansions (7) for this class
of operators. However, there are two available expansions, the divergences can be overcomed switching between the Weyl and Wigner representations.

The CZ index [24] is an integer function \( \nu_Q : t \in \mathbb{R} \geq 0 \mapsto \{0, 1, 2, 3\} \), whose vocation is to count how many times a path \( t \mapsto Q_t \in \text{Sp}(2n, \mathbb{R}) \) crosses the manifold \( \text{det}(Q_t - I_{2n}) = 0 \) and in which direction the crossing occurs, i.e., from negative to positive values or from positive to negative. This index and its companion \( \nu_{Q}^+ \) are defined through

\[
\sqrt{\text{det}(Q_t \pm I_{2n})} = i^{-\nu_Q} \sqrt{|\text{det}(Q_t \pm I_{2n})|}
\]

and both acquire the values in \( \{0, 2\} \) if \( \text{det}(Q_t \pm I_{2n}) > 0 \), or in \( \{1, 3\} \) if \( \text{det}(Q_t \pm I_{2n}) < 0 \). Note that the denominators in (39) and in (40) can be rewritten as (42).

If \( \hat{M}_S(\xi) \) and \( M_X(x) \) are both well-behaved, they are related by (11) and, for a given \( \nu_{S}^\pm \), the index \( \nu_S^\pm \) becomes

\[
\nu_S^\pm = \nu_{S}^\mp + \frac{1}{2} \text{Sng } C_S \quad \text{(mod 4),}
\]

where \( \text{Sng } X \) is the number of positive eigenvalues minus the number of negative eigenvalues of the matrix \( X \). Since both symbols does not diverge, then \( \text{det}(S \pm I_{2n}) \neq 0 \) and \( \text{Rank } C_S = 2n \), thus \( \frac{1}{2} \text{Sng } C_S \in \mathbb{Z} \) and \( \nu_{S}^\pm \in \{0, 1, 2, 3\} \). The Fourier relation (11) for the symbols in question should be faced as Fresnel-type integral [12].

From the above discussion, the main features of the CZ-index become clear: each of the two MOs (double coverage) associated to one symplectic matrix is distinguished by one value of the CZ-index, which in turn is associated to the sign of the square-root which appears in (39) or in (40); rather than mere signs, these indexes are imposed by the continuity of the operators when changing between representations by (43), or when a symbol crosses a divergence.

The CZ-index and some aspects of the MOs have been dealing here on a broader scope. However, in this work the treatment will focus only on the relationship between the uniparametric subgroups of \( \text{Sp}(2n, \mathbb{R}) \) and of \( \text{Mp}(2n) \) composed, respectively, by matrices of the form (23) and operators as in (38).3 The protocol for the Weyl–Wigner symbols of MOs in (38) which describes when symbols (39) and (40) attains a divergence will be briefly mentioned, inasmuch as all details and examples can be found in [34].

The continuity of an MO in (38) demands

\[
\lim_{t \to 0^+} S_t = I_{2n} \Rightarrow \lim_{t \to 0^+} \hat{M}_{S_t} = +\hat{1}.
\]

Thus, for \( t = 0 \), the Weyl symbol \( \hat{M}_{I_{2n}}(\xi) \) is not defined. However, the Wigner symbol of the identity operator should be \( \hat{M}_{I_{2n}}(x) = +1 \) from (44), which shows that \( \nu_{I_{2n}}^+ = 0 \). The imposition of the initial condition (44) restricts the values of the indexes throughout the whole evolution dictated by \( S_t \), Supposing that the two symbols (39) and (40) never diverge at the same instant, just before a divergence of one symbol, relation (11), or its inverse, should be used to determine the other. Thus after the same divergence, the original symbol is recovered also using the inverse, or the direct version, of (11). For each Fourier transformation, the appropriate CZ-index is determined by (43), and note that, out of a divergence, \( \text{Sng } C_{S_t} = \text{Sng } C_{S_t}^{-1} \).

3The complete representation theory between \( \text{Sp}(2n, \mathbb{R}) \) and \( \text{Mp}(2n) \) is developed in [12].
3.3. Inhomogeneous metaplectic group

The composition of a generic MO with the Heisenberg translation (5) is a direct consequence of (36):

$$\hat{M}_S \hat{T}_x \hat{M}_S^\dagger = \hat{T}_{\xi}. \quad (45)$$

This relation turns to be possible the definition of the inhomogeneous metaplectic group $\text{IMp}(2n)$ which is composed by operators of the form

$$\hat{U} = e^{\frac{i}{\hbar} \hat{T}_x \hat{M}_S}, \quad (46)$$

where $\hat{T}_x \in \mathcal{H}(2n), \hat{M}_S \in \text{Mp}(2n)$, and $\phi \in \mathbb{R}$.

An uniparametric subgroup of $\text{IMp}(2n)$ has its elements conveniently written as

$$\hat{U}_t = \hat{T}_\eta \hat{M}_S t \hat{T}_\eta^\dagger e^{-\frac{i}{\hbar} H_0 t}, \quad (47)$$

with $\hat{T}_\eta$ in (5), and $\hat{M}_S_t$ in (38). The above unitary operator is indeed a member of $\text{IMp}(2n)$, since $\hat{U}_t$ assumes the form in (46) when relations (45) and (32) are applied. Generators of this subgroup are determined through

$$\hat{H} := i\hbar \frac{d\hat{U}_t}{dt} = \frac{1}{2} \hat{x} \cdot \hat{H} \hat{x} + \hat{x} \wedge \eta + H_0', \quad (48)$$

which is the symmetric quantization of the Hamiltonian (25) with $\eta = -JH_0$ and $H_0' := H_0 + \frac{1}{2} \eta \cdot \hat{H}_J$, thus a member of $\text{IMp}(2n)$ Lie algebra [11, 12].

The Weyl symbol in (18) of the unitary operator in (47) is obtained using the composition rules of translations and reflections in section 3.1, the symplectic covariance relation (45), and the ciclicity of the trace. Indeed,

$$\tilde{A'}(\xi) = \text{Tr} \left( \hat{M}_S \hat{T}_\xi \hat{T}_\eta^\dagger \hat{M}_S^\dagger \right) e^{-\frac{i}{\hbar} H_0 t}$$

$$= \text{Tr} \left( \hat{M}_S \hat{T}_\eta^\dagger \hat{T}_\xi \hat{M}_S^\dagger \right) e^{-\frac{i}{\hbar} H_0 t - \frac{i}{\hbar} \xi \eta} \quad (49)$$

$$= \tilde{M}_S(\xi) e^{-\frac{i}{\hbar} (H_0 t + \xi \eta)},$$

where $\tilde{M}_S(\xi)$ is defined by (39). Similarly, the Wigner symbol becomes

$$U_t(x) = M_S(x - \eta) e^{-\frac{i}{\hbar} H_0 t}, \quad (50)$$

where $M_S(x)$ is defined by (40).

3.4. Covariances of operators and symbols

The covariance relation (45) is the one of, if not, the major advantage in working with a basis of operators which sets momentum and position on equal footing. Consider $Q \in \text{Sp}(2n, \mathbb{R}), \xi \in \mathbb{R}^{2n}$, and the operator defined as

$$\hat{A}' := (M_Q \hat{T}_\xi)^\dagger \hat{A} (M_Q \hat{T}_\xi). \quad (51)$$

Taking the Weyl–Wigner expansion of $\hat{A}$ in (7), by virtue of the composition formulas (32), (34) and of (45), the symbols are covariant with $A'$:

$$\tilde{A}'(\xi) := A(Q(\xi)) e^{\frac{i}{\hbar} \xi \cdot \hat{C}}, \quad A'(x) := A(Q(x + \xi)). \quad (52)$$
Applying the above covariance rule for the symbols of the MO (39) and (40), one finds

\[ M'_{S}(\xi) = M_{S}(Q\xi)e^{i\xi/Q}, \]

\[ M'_{S}(x) = M_{S}(Q(x + \zeta)) = M_{Q^{-1}S}(x + \zeta), \]

where the rightmost equalities in both equations are consequences of the covariance of the Cayley transform in (41),

\[ Q^\top C S Q = C Q^{-1} S Q, \]  

(53)

and of \( \det \left( Q^{-1} S \pm I_{2n} \right) = \det \left( S \pm I_{2n} \right) \). Since \( Q^\top C S Q \) is a congruence of \( C S \), thus

\[ \text{Sng} C_{S} = \text{Sng}(Q^{-1} C S Q) = \text{Sng} C_{Q^{-1} S Q}, \]  

(54)

The last invariance relations, by (42) and (43), also guarantee the invariance of the CZ index:

\[ \nu^\pm_{Q^{-1} S Q}(t) = \nu^\pm_{S}(t). \]

By the end, since \( Q^{-1} S Q \) is similar to \( S \), its eigenvalues are invariant.

If the evolution is governed by Hamiltonian (48), the unitary operator in (47), after the transformation in (51), becomes

\[ \hat{U}'_{t} = \hat{T}_{Q^{-1} \eta - \zeta} \hat{M}_{Q^{-1} S} \hat{T}_{Q^{-1} \eta - \zeta} e^{i\hat{H}_{0}t}. \]

The intrinsic relation of \( \hat{M}_{Q^{-1} S} \) in above formula with the metaplectic evolution in (38) is revealed by equation (36):

\[ \hat{M}_{Q^{-1} S} = \hat{M}_{Q}^\dagger \hat{M}_{S} \hat{M}_{Q} = \exp \left[ -i t \hat{x} \cdot Q^{-1} H Q \hat{x} \right], \]

which is the MO associated to covariant symplectic matrix

\[ S'_{t} = \exp(\hat{J} Q^{-1} H_{0} t) = \exp(\hat{Q}^{-1} J H_{0} t) = Q^{-1} S_{t} Q. \]

Since \( H' = Q^{-1} H_{0} Q \) and \( J H' = Q^{-1} J H_{0} Q \), then \( \text{Sng} H' = \text{Sng} H \) and the spectrum of \( J H \) are invariant, as well as the spectrum of \( S_{t} \).

4. Thermal operators of quadratic Hamiltonians

The Weyl–Wigner symbols of the thermal operator and the PF for a general QH will be calculated through the mathematical tools presented in all previous sections. Thermodynamical properties and the classical limit for the QHs will also be developed.

4.1. Weyl–Wigner representation

The Cayley parametrization (41) of the complex symplectic matrix in (28) is an anti-Hermitian matrix, since it is symmetric and

\[ \text{Re} C_{S,j} = 0 \iff C_{S,j}^\ast = C_{S,j}^{-1} = -C_{S,j}, \]  

(55)
due to the property in (30). The formula for $C_{S_{\beta}}$ can be manipulated to write it in terms of the real and complex components of $S_{\beta}$. Indeed, if $-\frac{1}{\beta} \notin \text{Spec}(S_{\beta})$, from (41) and using (30),

$$C_{S_{\beta}} = J^\top (\text{Re } S_{\beta} + I_{2n})^{-1} (S_{\beta}^* + I_{2n})(S_{\beta} - I_{2n})^{-1} (S_{\beta}^* + I_{2n})^{-1} (S_{\beta} - I_{2n})^{-1}$$

For the case in which $1 \notin \text{Spec}(S_{\beta})$, a similar procedure gives

$$C_{S_{\beta}}^{-1} = i(\text{Re } S_{\beta} - I_{2n})^{-1} (\text{Im } S_{\beta}) J^\top.$$ 

Note also that

$$\det C_{S_{\beta}} = (-1)^n \det \text{Im } C_{S_{\beta}} \in \mathbb{R}, \quad \det(S_{\beta}^* \pm I_{2n}) = \det(S_{\beta}^* \pm I_{2n}) = \det(S_{\beta} \pm I_{2n}) \in \mathbb{R},$$

and remember that the action of the Wick rotation preserves the categorization of the eigenvalues, see equation (31).

The Weyl symbol of the thermal operator $\exp[-\beta \hat{H}]$ for the Hamiltonian (48) is readily determined by the mapping (20) of the symbol (49),

$$\tilde{E}_{\beta}(\xi) = e^{-\frac{1}{2}\hbar \xi \cdot J(\text{Im } C_{S_{\beta}})} e^{-\frac{1}{2}\hbar \xi \cdot \eta}, \quad (57)$$

and of the Wigner symbol (50),

$$E_{\beta}(x) = 2^n e^{\frac{i}{\hbar} \text{Im } C_{S_{\beta}}(x - \eta) - \beta H_0} \sqrt{\det(S_{\beta} \pm I_{2n})}, \quad (58)$$

As before, the Fourier transformation links above symbols when both are well behaved, i.e., when $\pm 1 \notin \text{Spec}(S_{\beta})$. However, the convergence of (11) now is more restrictive, since $\text{Im } C_{S_{\beta}} \in \text{Mat}(2n, \mathbb{R})$. It will be only guarantied if the integrand in (11) is an absolutely integrable function [27]. For the symbols in question, this means $\text{Sng } \text{Im } C_{S_{\beta}} = -2n$, that is, if $\text{Im } C_{S_{\beta}} < 0$. This further requirement is a consequence of the mentioned matrix being real, and thus the integration does not rely any more on a Fresnel prescription, as it was before. Furthermore, the indexes defined through (42) are mapped naturally by (3) to

$$\sqrt{\det(S_{\beta} \pm I_{2n})} = i^{-\nu_{S_{\beta}}^+} \sqrt{\det(S_{\beta} \pm I_{2n})}, \quad (59)$$

also subjected to a physical ‘initial condition’:

$$\lim_{\beta \to 0^+} S_{\beta} = I_{2n} \Rightarrow \lim_{\beta \to 0^+} e^{-\beta \hat{H}} = +1. \quad (60)$$

Considering thus that all the requirements are met, the Fourier transformation gives

$$\nu_{S_{\beta}}^+ = \nu_{S_{\beta}}^-. \quad (61)$$
From equation (17), the characteristic and Wigner functions of a thermal state of a QH are, respectively,
\[
\chi(\xi) = \frac{e^{-\frac{i}{\hbar} J(\mathrm{Im} C_{\beta,\eta})^{-1} J_{\xi - \beta H_0}}}{(2\pi\hbar)^{n}},
\]
\[
W(x) = \frac{e^{\frac{i}{\hbar} (x-\eta) J \mathrm{Im} C_{\beta,\eta}(x-\eta)}}{(\pi\hbar)^n \sqrt{\det \mathrm{Im} C_{\beta,\eta}^{-1}}}.
\]
(62)

If $\mathrm{Im} C_{\beta,\eta} < 0$, the Wigner function will be a normalized Gaussian with covariance matrix $\frac{1}{2} \mathrm{Im} C_{\beta,\eta}^{-1}$ and mean-value $\eta$, this condition is satisfied only by Hamiltonians in category (E), see section 6.4.

Otherwise, the Wigner function is not defined, since it will not provide the correct probability marginals of the quantum state [10]. However, the thermal operator can still be represented through its symbols in (57) and (58), or even by its characteristic function, since none of these are subjected to the expected properties of a genuine Wigner function.

The Cayley transform (41) can be uniquely inverted, if $-1 \notin \mathrm{Spec}(S) \beta$, to give
\[
S_{\beta} = (1_{2n} + J\mathbf{C}_{\beta,\eta})(1_{2n} - J\mathbf{C}_{\beta,\eta})^{-1},
\]
and a similar relation can be written when $1 \notin \mathrm{Spec}(S) \beta$. At the end of the day, there is only one symmetric matrix, $\mathrm{Im} C_{\beta,\eta} = -iS_{\beta,\eta}$, or its inverse, associated to one $S_{\beta} \in \mathbb{W} \mathrm{Sp}(2n, \mathbb{C})$. The dimension of the set of symmetric matrices in Mat$(2n, \mathbb{R})$ is $n(2n + 1)$ and is equal to the dimension of $\mathbb{W} \mathrm{Sp}(2n, \mathbb{C})$, since this is the dimension of its Lie algebra $\mathfrak{sp}(2n)$. Consequently, apart from the translation $\eta$ and the constant $H_0$, the symbols in (57) and (58) are uniquely specified by one matrix $S_{\beta}$. This should be compared with the case of the set of pure Gaussian states [11]. One Wigner function of this set is written exactly as (62), but replacing $\mathrm{Im} C_{\beta,\eta} \rightarrow -SS^\dagger$, with $S \in \mathbb{Sp}(2n, \mathbb{R})$. The dimension of the set of Wigner functions (without translations) is $n(n + 1)$, thus, smaller than the dimension of $\mathfrak{sp}(2n)$.

Including the translations with $\eta \in \mathbb{R}^{2n}$ and the constant $H_0 \in \mathbb{R}$, the dimension of the set of symbols of a thermal operator is $(n + 1)(2n + 1)$, corresponding to the dimension of $\text{Im}(2n)$, thus a symbol is completely determined by one Hamiltonian in (25).

For completeness, consider now the case of a linear Hamiltonian $H_1 = \hat{x} \wedge \eta$, which generates Weyl operators $T_{\eta,\hat{x}} \equiv \exp[-i/\hbar \hat{x} \wedge \eta t]$. From (20) and (35), the Wigner symbol becomes $E_\beta(x) = \exp[-i/\hbar \hat{x} \wedge \eta t]$. Since Wigner and Weyl symbols are related by the Fourier transformation (11), the Weyl symbol does not exist (note that such an exponential function $E_\beta(x)$ is not absolutely integrable). By other side, the use of (20) for the symbol $T_{\eta,\hat{x}}(\xi)$ from (35) generates an ill-defined Dirac delta function.

4.2. Covariance of symbols

Under the transformation (51), the symbols of the thermal operator behaves as (52), i.e.,
\[
E'_\beta(\xi) = \frac{e^{\frac{i}{\hbar} \xi\beta \mathbf{C}_{\beta,\eta}^{-1}\xi - \beta H_0}}{\sqrt{\det(S'_\beta - 1_{2n})}} \cdot e^{\chi'_{C_{\eta,\xi}}} \cdot \frac{e^{\frac{i}{\hbar} (\xi - \beta H_0)J - \beta H_0}}{\sqrt{\det(S'_\beta + 1_{2n})}},
\]
(63)
where
\[ S'_\beta = e^{-i\hbar/\beta JQ} H Q = e^{-i\hbar/\beta JH} Q^{-1} S_{\beta} Q. \] (64)

Noting that \( \det(S'_\beta \pm I_{2n}) = \det(S_{\beta} \pm I_{2n}) \) and, from equation (53), that \( \text{Sng}(\text{Im} C_{S'_\beta}) = \text{Sng}(\text{Im} C_{S_{\beta}}) \), the indexes (59) are invariant, i.e., \( \nu^\pm_{S'_\beta} = \nu^\pm_{S_{\beta}} \).

### 4.3. Partition function and indexes

The PF in (16) for the thermal state in question becomes
\[ Z_\beta = \frac{e^{-\beta H_0}}{\sqrt{\det(S_{\beta} - I_{2n})}}, \] (65)
which is trivially invariant under the transformation (64), since the trace of an operator is invariant under an unitary similarity.

Due to the equality of the indexes in (61), both ways of calculation in (16) are completely equivalent, expressing the fact that the trace of an operator is basis-independent. Remarkably, \( \lim_{\beta \to 0} S_{\beta} = I_{2n} \) is the high temperature limit and, as physically expected, the PF diverges for any Hamiltonian (48). It should be clear that this divergence is not a consequence of the chosen representation, as the ones which may happen for the symbols in (57) and (58). However, note that in the same limit \( \hat{E}_\beta(\xi) \) is not defined, while \( E_\beta(x) \) is a decreasing function due to \( C \rightarrow 0_{2n} \), see equation (41). Other divergences of (65) can occur when \( S_{\beta} \) has at least an eigenvalue equal to \( +1 \), this reflects structural properties of the system Hamiltonian, and will be investigated in the examples given in next section. Naturally there is no dependence on \( \eta \) in equation (65), since this term, the linear part of the Hamiltonian (48), is only a displacement of the fixed point ‘\( \hat{x} = 0 \)’ of the quadratic part.

Since \( \hat{H} \) is Hermitian, the PF is the trace of a positive operator, thus \( Z_\beta > 0 \). This is an extra requirement to the indexes in (59) besides equation (61). Practically, in calculations, this can be faced as redefining (65) to \( |Z_\beta| \), see equation (56). The indexes in equation (59) and the symbols in (57) and (58) sustain a double cover representation between the group \( \text{WSp}(2n, \mathbb{C}) \) and the set of thermal operators. This relation is inherited from the one between \( \text{Sp}(2n, \mathbb{R}) \) and \( \text{Mp}(2n) \).

The imposition of the index by the positivity of the PF has some physical and mathematical consequences. As another feature of the CZ-index, the composition of two MOs [11, 12] is such that \( M_{S_1} M_{S_2} = \pm M_{S_2} S_1 \), but only one sign in ‘\( \pm \)’ is correct if \( M_{S_1}, M_{S_2} \), and their respective CZ-index are determined. The correct sign of the product is itself given by a CZ-index, which is a function of the CZ-indexes of each MO and of all the involved symplectic matrices \( S_1, S_2, S_1 S_2 \) [12]. The choice made for the sign of the PF inhibits the interpretation of the set of thermal operators as a group, since the composition of such two operators is not guaranteed to be correct without a correct index treatment.

### 4.4. Thermodynamical properties

The PF is the first step toward the derivation of thermodynamical quantities [1]. To this end, consider the Jacobi formula [28] for the derivative of the determinant of an invertible matrix:
\[ d(\det A) = (\det A) \text{Tr}[A^{-1} \text{d}A]. \] (66)
This will show that all the thermodynamical functions will depend only on the eigenvalues of the Hamiltonian matrix \( JH \) or on the respective eigenvalues of \( S_{\beta} \), since \( Z_\beta \) is a function only of
the eigenvalues of $S_\beta$ through the determinant in (65). This determinant also guarantees that $Z_\beta$ is a product of partitions functions of each eigenvalue of $S_\beta$, thus extensive. In the following, the case (P) is excluded, since $(S_\beta - l_{2n})$ and $J H$ are singular matrices, see section 6.1 for this case.

The Helmholtz free energy of the system is

$$ F := -\frac{1}{\beta} \ln Z_\beta = H_0 + \frac{1}{2\beta} \ln |\det(S_\beta - I_{2n})|, $$

while the internal energy becomes

$$ U := -\frac{\partial}{\partial \beta} \ln Z_\beta = H_0 + \frac{\hbar}{4} \text{Tr}[H \text{Im} C^{-1}_{S_\beta}]. $$

The entropy is readily determined through the use of above formulas: $S = k_B \beta (U - F)$. Finally, the heat capacity is

$$ C := k_B \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z_\beta = -\frac{1}{2} k_B \hbar^2 \beta^2 \text{Tr}\left[ (JH)^2 \frac{S_\beta}{(S_\beta - I_{2n})^2} \right]; $$

the complex condition (30) can be used to certify that $C^* = C$, thus real. Needless to say, the mentioned thermodynamical quantities, and any other derived from them, are invariant under (64).

4.5. Classical limit

It is convenient to write the Hessian in (25) as $H = \varpi H_{\#}$, where $H_{\#}$ is a dimensionless matrix and $\varpi$ a characteristic frequency of the system. Thus, it is possible to write $H' = \frac{\varpi}{\hbar} x' \cdot H_{\#} x'$ and by the covariance properties, nothing changes except the system of units. As matter of simplicity, the symbol $\#$ will be forgot and the classical (high temperature) limit becomes simply expressed as $\beta := \hbar \varpi / \beta \ll 1$.

In this limit, expanding $S_\beta$ in (28), there is no even-order corrections to the Cayley matrix (41):

$$ C_{S_\beta} = -\frac{i}{2} \beta H + \frac{i}{24} \beta^3 (JH)^3 + O(\beta^5), $$

since it is an anti-Hermitian matrix, see equation (55). However, with the help of (66)

$$ [\det(S_\beta + I_{2n})]^{-1} = \frac{1}{2^n} \left[ 1 - \frac{1}{16} \beta^2 \text{Tr}(JH)^2 \right] + O(\beta^4). $$

Consequently, the Wigner symbol (58) approximates to

$$ E_\beta(x) \approx \left[ 1 - \frac{\beta^2}{16} \text{Tr}(JH)^2 \right] \exp[-\beta H_{cl}], $$

4 Assuming that every quantity is measured in the SI, consider the symplectic matrix $U = (\sqrt{kg} s^{-1} l_{2n}) \oplus (\sqrt{s} kg^{-1} l_{2n})$, which corresponds to a change of units. The transformed vector $x' = U x$ is composed by coordinates and momenta both measured in $\sqrt{kg} m^2 s^{-1}$, i.e., both with the same unit of $\sqrt{\hbar}$. In this system of units, all the elements of the Hessian $H$ in equation (25) are measured in $s^{-1}$ to keep the Hamiltonian in Joules. Note that this is necessary to correct write the units of the thermodynamical quantities, see for instance equation (68).
which is equal to the Boltzmann factor of the classical Hamiltonian (25) if the second order corrections are discarded.

In the same limit, putting the expansion of $S_\beta$ in (68) and in (69), the internal energy and the heat capacity of the system are given, respectively, by

$$ U = H_0 + n\beta^{-1} - \frac{\hbar\omega}{4!} \beta \text{Tr}(JH)^2 + \mathcal{O}(\beta^3), $$

(71)

$$ C_v = nk_B + \frac{\hbar^2}{4!} \beta^2 \text{Tr}(JH)^2 + \mathcal{O}(\beta^4). $$

Both above formulas express the equipartition theorem [1] for a generic QH if all higher order corrections in $\beta$ are neglected.

5. General Hamiltonians

The symbols of a thermal operator for a generic Hamiltonian can be obtained using the Wick mapping (20) of the symbol of the corresponding unitary operator. However, there are few cases in which the symbol of an unitary operator can be analytically settled. Fortunately, semiclassical methods can help in determine properties of such generic thermal operators.

The only situations where the (normalized) Wigner symbol $\hat{H}(x) := \text{Tr}(HR_x)$ of a quantum Hamiltonian $\hat{H}$ is equal to the classical Hamiltonian $H_\text{cl}$ are the quadratic case in (48) [11], the separable case $\hat{H} = T(\hat{p}) + V(\hat{q})$ [10], and either a combination of both. For a generic quantum system, the (normalized) Wigner symbol of the Hamiltonian is a smooth function which tends to the classical value in the limit $\hbar \to 0$ [10]. The (normalized) Wigner symbol of powers $\hat{H}^k$ of the Hamiltonian, $\hat{H}^k(x) := \text{Tr}(\hat{H}^kR_x)$, is obtained by the Groenewold formula [32],

$$ \hat{H}^k(x) = e^{\frac{i}{\hbar} \frac{\partial^k}{\partial x^k} \hat{H}(x_1)\hat{H}^{-1}(x_2)} |_{x_1 = x}, $$

(72)

which is no longer factorisable into individual symbols. However, since the Weyl symbol of a Hermitian operator is real, the recursive expansion of the above exponential shows that

$$ \hat{H}^k(x) = [H(x)]^k + \mathcal{O}(\hbar^2), $$

(73)

i.e., the symbols of powers of the Hamiltonian differs from the power of the symbol only in second order in $\hbar$. For $k = 2$, it will be useful to go one order further in the expansion of equation (72) to find

$$ \hat{H}^2(x) = [H(x)]^2 - \frac{\hbar^2}{8} \text{Tr}(J \partial_x^2 H)^2 + \mathcal{O}(\hbar^4). $$

(74)

Note that all odd powers in the expansion of (72) are null, since the Wigner symbol of any Hermitian operator is real, see equation (15).

In the crude semiclassical limit, $\hbar \to 0$, square and higher powers of $\hbar$ can be discarded in (73). Furthermore, the Taylor expansion of the thermal operator $e^{-\beta H}$ and the linearity of the trace are enough to write

$$ \hat{E}_\beta(x) := \text{Tr}(e^{-\beta H}R_x) = \sum_{k=0}^{\infty} \frac{(-\beta)^k}{k!} \hat{H}^k(x) \approx e^{-\beta H(x)}, $$

(75)

Note the absence of the factor $2^n$ in this definition when compared to the one in equation (8).
due to equation (73). In this limit, the symbol $\hat{H}(x)$ gets arbitrarily closer to the classical Hamiltonian of the system $H_{cl}$, which shows that $\bar{E}_\beta(x)$ approaches to the classical Boltzmann factor.

The semiclassical approximation in [10], which is the core of the one realized here, involves the expansion of the unitary operator (2) in powers of $t/\hbar$, which restricts the convergence to small time intervals. Consequently, the composition of Wigner symbols of the unitary operator for small steps is necessary to construct an approximation valid for any time. Since the expansion for the thermal operator itself in (75) does not involves $\hbar$, the approximation is valid for any value of $\beta$.

A subtle distinction occurs when including the term in $\hbar^2$ from equation (74) into the expansion (75). Recalling the unity change in section 4.5, which here is accomplished by $\bar{H}(x) \rightarrow \bar{H}_0(x)$, the mentioned term will be the unique contribution of order $\bar{H}_0^2 := \bar{\omega}^2 \beta^2 \hbar^2$ to the sum in (75), i.e.,

$$\bar{E}_\beta(x) = e^{-\beta \bar{H}(x)} - \frac{\beta^2}{16} \text{Tr}(J \partial^2_{xx} \bar{H})^2 + \mathcal{O}(\beta^4 / \hbar),$$

and can be rewritten as

$$\bar{E}_\beta(x) = \left[ 1 - \frac{\beta^2}{16} \text{Tr}(J \partial^2_{xx} \bar{H})^2 \right] e^{-\beta \bar{H}(x)} + \mathcal{O}(\beta^4 / \hbar),$$

since this last cannot be distinguished from the former in order of $\beta^4$ [10]. In the high temperature limit, higher order powers of $\beta$ are discarded, and $\bar{E}_\beta(x)$ approaches the Boltzmann factor of the (normalized) Wigner symbol of the Hamiltonian $\hat{H}$. If $\hat{H}$ is the QH in (48), then the limit (70) is recovered, since $\hat{H}(x) = \text{Tr}(\hat{H} \hat{R}_x)$ is equal to $H_{cl}$ in (25).

The behavior of the system around a critical (fixed) point of the symbol $\bar{H}(x)$ in the semiclassical or in the high temperature limits is circumscribed to one of those classical categories (P, H, E and L), thus mimicking the examples which will be presented in section 6. Supposing the existence of $x_0 \in \mathbb{R}^2$ such that $\partial_x \bar{H}(x) = 0$, the ‘Hamiltonian’ $\bar{H}(x)$ can be approximated to

$$\bar{H}(x) \approx \bar{H}(x_0) + \frac{1}{2}(x - x_0) \cdot \bar{H}_0(x - x_0), \quad \bar{H}_0 := \partial^2_{xx} \bar{H}(x_0),$$

for small enough $\delta x : = |x - x_0|$. Inserting this expansion in (76), one obtains

$$\bar{E}_\beta(x) \approx \left[ 1 - \frac{\beta^2}{16} \text{Tr}(J \bar{H}_0)^2 \right] e^{-\beta \bar{H}_0(x)} + \mathcal{O}(\beta^4 \delta x^3 / \hbar),$$

which is exactly formula (70), since

$$H^0_{cl} := \frac{1}{2} x \cdot \bar{H}_0 x + x \wedge x_0 + \bar{H}(x_0).$$

In principle a Wick rotation could be applied to obtain approximations for the thermal operator from the well established formulas of semiclassical approximations for unitary operators. This route was not adopted since some kinds of semiclassical approximations, for instance the one in [11, 33], necessarily approximates time-independent Hamiltonians by time-dependent ones. Such rotation when applied to a time-dependent Hamiltonian generates a temperature-dependent one.
6. Examples of quadratic Hamiltonians

The Hamiltonians for the following examples were in majority retrieved from the list of normal-form Hamiltonians in [23], which is itself a compilation of the results in [29]. All the systems of that list can be worked out in the lines presented here. However some of them, specially degenerate systems in higher dimensions, may require numerical calculations for the determination of the eigenvalues of the corresponding Cayley parametrization. By another side, this trouble can be circumvented in specific cases, see for instance section 6.3. The determination of the PF and/or the thermodynamical quantities in section 4.4 relies only on the eigenvalues of \(J_H\), i.e., the Cayley matrix is not needed for the obtainment of these quantities.

The term ‘normal-form’ indicates the simpler form which a generic QH, like (22), can be brought by a symplectic transformation. Indeed, for any \(S \in \text{Sp}(2n, \mathbb{R})\), the symplectic transformation \(x' = Sx\) changes (25) to

\[
H'_{\text{cl}} = \frac{1}{2} x' \cdot H x' + x' \wedge \zeta + H_0
\]

\[
= \frac{1}{2} Sx \cdot HSx + Sx \wedge \zeta + H_0 \quad \text{(E-1)}
\]

however, the Hamiltonian matrix of the new Hamiltonian \(H'_{\text{cl}}\) becomes similar to the old one

\[
JH' = JS^\top HS = S^{-1}(JH)S. \quad \text{(E-2)}
\]

Thus, following [29], it is possible to suitably choose \(S\), such that \(JH'\) has one of the normal forms in [23]. These normal forms constitute the building blocks, which combined generate all QHs. Note that (E-1) is accomplished in the quantum case by the covariance relations in section 3.4, and the consequences of (E-1) and (E-2) are readily translated for thermal states as in (63) and (64).

6.1. Parabolic Hamiltonian

The most known example of a Hamiltonian in category (P) is the free particle. One generic Hamiltonian of an \(n\) degrees-of-freedom system in (P) is the one having only kinetic energy. The Hessian (22) of such a Hamiltonian is

\[
H = 0_n \oplus M, \quad M \in \text{Mat}(n, \mathbb{R}). \quad \text{(E-3)}
\]

The Hamiltonian matrix and the symplectic matrix for this Hamiltonian becomes

\[
JH = \begin{pmatrix} 0_n & M \\ 0_n & 0_n \end{pmatrix}, \quad S_t = I_{2n} + JHt = \begin{pmatrix} I_n & Mt \\ 0_n & I_n \end{pmatrix}.
\]

Note that eigenvalues of \(JH\) are all null and the ones of \(S_t\) are all one, which justify the categorization of this system as (P), thus

\[
\det(S_t - I_2) = 0, \quad \det(S_t + I_2) = 2^{2n} \quad (\forall \ t > 0). \quad \text{(E-4)}
\]

Consequently, there is no divergence for the Wigner representation (39) of the MO, while there is absolutely no Weyl representation (40). The Cayley parametrization (41) becomes

\[
C_{S_t} = 0_n \oplus \frac{1}{2} Mt
\]
and the equation (44) sets $\nu_{\beta_{0}}^{+}(t) = 0$, $\forall t > 0$. Collecting all these results, the Wigner symbol for the MO associated to the free particle Hamiltonian is

$$M_{S_{\nu}}(x) = \exp \left[ -\frac{i t}{2\hbar} p \cdot M p \right].$$

(E-5)

Considering the thermal operator for the same Hamiltonian, the complex symplectic matrix in (28) becomes

$$S_{\beta} = I_{2n} - i\hbar \beta J H.$$

Since the eigenvalues are preserved by the Wick mapping, see equation (31), $\det(S_{\beta} - I_{2}) = 2^{2n}$, $\forall t > 0$, as in (E-4). The Cayley parametrization (41) for $S_{\beta}$ is

$$C_{S_{\beta}} = 0_{n} \oplus \left( -\frac{i}{2} M \hbar \beta \right),$$

and, accordingly to (60), $\nu_{S_{\beta}}^{+} = 0$.

The Wigner symbol in (58) becomes

$$E_{\beta}(x) = \exp \left[ -\frac{\beta}{2} p \cdot M p \right],$$

which is simply the Wick mapping (3) applied to (E-5).

Since $\det(S_{\beta} - I_{2}) = 0$, $\forall t > 0$, there is no Weyl representation for the thermal operator, as before. However, the matrix $\text{Im} C_{S_{\beta}}$ is negative-semidefinite for a positive-definite $M$. Pushing the luck, this is enough to guarantee the convergence of the Fourier integral (11) of the Wigner symbol in the momentum space, while in coordinate space, a delta distribution is used:

$$E_{\beta}(x) = \int_{\mathbb{R}^{n}} d^{n}q \int_{\mathbb{R}^{n}} d^{n}p \ e^{-\frac{i}{\hbar} q \cdot M p} \ e^{\frac{\beta}{2} q \cdot M^{-1} q}$$

$$\left(2\pi\hbar\right)^{n} \delta^{n}(\xi_{0}) \ exp \left[ -\frac{\xi_{0} \cdot M^{-1} \xi_{0}}{2\hbar^{2}\beta} \right].$$

The PF in (65) is divergent, since $\det(S_{\beta} - I_{2}) = 0$. Note that, from above Weyl symbol, $E_{\beta}(0)$ is a delta-function. However, it is customary in statistical physics to force a convergence by truncation of integrals like the one in (16). This is accomplished for the presented example considering the integral in configuration space as the volume $V$ occupied by the system:

$$Z_{\beta} = \int d^{n}q \int d^{n}p \ e^{\frac{\beta}{2} q \cdot M p} \left(2\pi\hbar\right)^{n} \sqrt{\det M} \left(2\pi\hbar^{-2}\beta\right)^{n} \delta^{n}(\xi_{0}) \ exp \left[ -\frac{\xi_{0} \cdot M^{-1} \xi_{0}}{2\hbar^{2}\beta} \right].$$

(E-6)

Consider now a rotation in phase space $x' = J x$. The new Hamiltonian $H' = \frac{1}{2} q \cdot M q$ has Hessian

$$H' = J \top H J = M \oplus 0_{n}.$$

From the covariance relation (63), the Wigner symbol in (58) becomes

$$E'_{\beta}(x) = \exp \left[ -\frac{\beta}{2\hbar} \frac{q}{2} \cdot M q \right],$$

which is simply the Wick mapping (3) applied to (E-5).
with $\nu^+_{\beta} = \nu^+_{\beta} = 0$, see section 4.2. The Fourier transformation of above symbol gives

$$\tilde{E}'_{\beta}(\xi) = \frac{(2\pi)^n}{\sqrt{\det M}} \delta(\xi_q) \exp \left[ -\frac{\xi_p \cdot M^{-1} \xi_p}{2\hbar^2 \beta} \right].$$

The PF is again obtained by integrating the Wigner symbol $E'_{\beta}(x)$, however the convergence now is performed truncating the momenta-integral, and becomes

$$Z_{\beta} = \int_{\mathbb{R}^n} d^p \int_{\mathbb{R}^n} d^q \frac{E'_{\beta}(x)}{(2\pi\hbar)^n} = \frac{\mathcal{V}'}{(2\pi\hbar^2 \beta)^{n^2}} \sqrt{\det M},$$

where $\mathcal{V}'$ is the volume of momenta space. Due to the truncation performed, $Z_{\beta}$ is not invariant under the symplectic transformation $x' = Jx$, as it should be.

Concluding, the procedure to obtain the symbols and the thermodynamical properties of system in category (P) departs from the obtainment of the symbol $E_{\beta}(x)$, and then the PF through a truncation of the integrals, which can be independently either on momenta or coordinates, or even in a mixture of both. Formulas in section 4.4 do not work, and the thermodynamical functions should be derived directly for PFs as in the standard literature [1].

### 6.2. Hyperbolic Hamiltonian

The one degree of freedom normal-form Hamiltonian in category (H) is $H_0 = \kappa pq$ [23]. In quantum optics, its symmetric quantized version, $\hat{H} = \frac{\kappa}{2}(\hat{q}\hat{p} + \hat{p}\hat{q})$, is responsible for the phenomenon of squeezing [14].

The Hessian, the Hamiltonian matrix and the symplectic matrix for the Hamiltonian are

$$H = \kappa \sigma_x, \quad JH = \kappa \sigma_z, \quad S_t = \text{Diag}(e^{\kappa t}, e^{-\kappa t}),$$

where $\sigma_x$ and $\sigma_z$ are the Pauli matrices. The complex symplectic matrix (28) is, thus,

$$S_{\beta} = \text{Diag}(e^{-i\bar{\beta}}, e^{i\bar{\beta}}), \quad \bar{\beta} := \hbar \kappa \beta.$$

As stated in (31), the eigenvalues of $JH$ (and of $S_t$) classifies this matrix as (H), and the Wick rotation generates a matrix $S_{\beta}$ in (E).

The Cayley parametrization (41) for $S_{\beta}$ is

$$C_{S_{\beta}} = -i \text{tg} \left( \frac{\beta}{2} \right) \sigma_x,$$

and

$$\det(S_{\beta} - I_2) = 4 \sin^2 \left( \frac{\beta}{2} \right), \quad \det(S_{\beta} + I_2) = 4 \cos^2 \left( \frac{\beta}{2} \right).$$

The Weyl symbol in (57), using equations (59), (E-7) and (E-8), becomes

$$\tilde{E}_{\beta}(\xi) = \frac{i\nu^+_{\beta}}{2} \csc \left( \frac{\beta}{2} \right) \exp \left[ -\frac{1}{2\hbar} \text{ctg} \left( \frac{\beta}{2} \right) \xi_q \xi_p \right].$$
and is not defined when $\bar{\beta} = h\kappa\beta = m\pi$, for $m \in \mathbb{N}$. The Wigner symbol (58) is expressed as

$$E_\beta(x) = i^{\nu_\beta} \left| \frac{\bar{\beta}}{2} \right| \exp \left[ -\frac{2}{h} \tan \left( \frac{\bar{\beta}}{2} \right) x p \right],$$  

(E-10)

and is not defined when $\bar{\beta} = h\kappa\beta = (2m + 1)\pi$, for $m \in \mathbb{N}$. The PF (65) obtained through $\tilde{E}_\beta(0)$ is

$$Z_\beta = i^{\nu_\beta} \left| \csc \left( \frac{\bar{\beta}}{2} \right) \right|.$$  

(E-11)

It remains to determine the indexes in (E-9), in (E-10), and in (E-11). From equation (E-7), $\text{Spec(Im } C_{\beta,\beta} \text{)} = \{ \pm \operatorname{tg}(h\kappa\beta/2) \}$, consequently neither (E-9) nor (E-10) are (absolutely) integrable functions, which inhibits the Fourier transformation (11) among the symbols. However, the PF is the trace of a positive operator, thus it is positive, which gives $\nu_{\beta,\beta} = 0, \forall \beta \geq 0$. From (60), $\lim_{\beta \to 0} E_\beta(x) = 1$ and thus, taking into account the first divergence of (E-10), $\nu_{\beta,\beta} = 0$ for $0 < h\kappa\beta < \pi$, and this is the only interval where it is possible to determine $\nu_{\beta,\beta}$, due to the absence of a Fourier transformation. By the same reasons, the Wigner function (62) for the thermal state of the hyperbolic Hamiltonian is not defined, but the chord function is given also in (62) with (E-7).

The heat capacity for this Hamiltonian, from (69), is

$$C = \frac{1}{4} k_B \beta^2 \csc^2 \left( \frac{\bar{\beta}}{2} \right),$$

and is plotted in figure 1, where it is also shown the PF of the system. Both functions diverges for $\bar{\beta} = \bar{\beta}_c = 2m\pi$, and expanding the above formula around these values, one obtains a critical exponent $\alpha = 2$. However, in the present situation, this divergence is a pure mechanical effect and cannot be faced as a kind of phase transition, since the internal energy (68) and the free-energy (67) are themselves discontinuous at the same points. Note that $\lim_{\beta \to 0} C = k_B$ in agreement with (71).

The scattering of a particle through a parabolic barrier is described by inverted oscillator $H' = \kappa^2 (p^2 - q^2)$, which is a rotation of the hyperbolic Hamiltonian considered, i.e., $H'_{cl} = H_{cl}(R)$, where

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \in \text{Sp}(2, \mathbb{R}).$$

The symbols of the thermal operator for the inverted oscillator are readily obtained using the covariance relations (63), while the PF, since it is invariant, is the same as (E-11).

As an observation, similar to what was done in equation (E-6) for the configuration space, an attempt to truncate the integration of (E-10) in position and either in momentum, constraining the system to a phase space volume $\Omega$, attain

$$Z_\beta = \frac{1}{\pi} \csc \left( \frac{\bar{\beta}}{2} \right) \left| \text{Shi} \left[ \frac{2\Omega}{h} \tan \left( \frac{\bar{\beta}}{2} \right) \right] \right|,$$  

(E-12)

and does not remove the divergences of the PF.

As a last comment, it should be also noted that, since all the thermodynamical quantities are functions exclusively of the eigenvalues of $\tilde{S}_\beta$, or the ones of $\mathbf{JH}$, their behavior is a property of the whole class of systems in category (H).
Figure 1. PF (Left) and the heat capacity (Right) of the Thermal state for the one degree of freedom hyperbolic Hamiltonian $H(x) = \kappa pq$ as a function of the inverse temperature $\tilde{\beta} := \hbar \kappa \beta$.

6.3. Degenerate hyperbolic Hamiltonian

From the generality of the QHs, it is interesting to work on a nontrivial system dynamics. The normal-form Hamiltonian of a system with $n$ degrees of freedom and $n$-fold degenerate pairs of eigenvalues $(\kappa, -\kappa)$ in category (H) is [23]

$$H_{cl} = \kappa \sum_{j=1}^{n} p_{j}q_{j} - \kappa \sum_{j=1}^{n-1} p_{j}q_{j+1},$$

which reduces to the case of previous example for $n = 1$. The Hessian of the Hamiltonian is

$$H = \begin{pmatrix} 0 & K \\ K^\top & 0 \end{pmatrix}, \quad K := \kappa (I_n - N),$$

(E-13)

and $N \in \text{Mat}(n, \mathbb{R})$ is the nilpotent matrix with entries $N_{jl} := \delta_{j,l+1}$. The Hamiltonian matrix becomes

$$JH = K^\top \oplus (-K),$$

and generates the complex symplectic matrix, via (28),

$$S_{\beta} = (e^{-i\beta} e^{iN^T}) \oplus (e^{i\beta} e^{-iN}), \quad \tilde{\beta} := \hbar \kappa \beta,$$

(E-14)

where

$$e^{N\alpha} = \sum_{j=0}^{n-1} \frac{\alpha^j}{j!} N^j = \begin{pmatrix} 1 & \frac{\alpha}{2} & \ldots & \frac{\alpha^{n-1}}{(n-1)!} \\ 0 & 1 & \alpha & \ldots \\ 0 & 0 & 1 & \ldots \\ \vdots & \vdots & \vdots & \alpha \\ 0 & \ldots & 0 & 1 \end{pmatrix}.$$ 

Due to the triangular structure of the blocks of $S_{\beta}$, it is not difficult to show that its $n$-fold degenerate spectrum is $\{\exp(-i\tilde{\beta}), \exp(i\tilde{\beta})\}$, thus
\[
\det(S_β - I_{2n}) = 2^{2n} \sin^2 \left( \frac{\beta}{2} \right),
\]
\[
\det(S_β + I_{2n}) = 2^{2n} \cos^2 \left( \frac{\beta}{2} \right).
\]

From these two, the symbols \( \tilde{E}_β(\xi) \) and \( E_β(\xi) \) diverges, respectively, as in (E-9) and as in (E-10).

An explicit expression for the Cayley parametrization (41) of \( S_β \) involves lots of cumbersome expressions, however, it is possible to write
\[
C_{S_β} = \begin{pmatrix}
0_n & -[F(N)]^* \\
F(N) & 0_n
\end{pmatrix}.
\]

(E-15)

Taking advantage of the nilpotency of \( N \), the function \( F \) can be represented as a finite power series:
\[
F(N) := [e^{iβN} + e^{-iβI_n}]^{-1}[e^{iβN} - e^{-iβI_n}]
\]
\[
= \sum_{m=0}^{n-1} \frac{N^m}{m!} \partial^m F(N),
\]
which can be easily computed in any symbolic computational software. Since a general analytic expression for \( C_{S_β} \) is missing, the determination of the eigenvalues of \( \text{Im} C_{S_β} \) is impossible. However, its characteristic polynomial, from (E-15), is
\[
P(λ) = \det \left[ λI_{2n} - \text{Im} C_{S_β} \right]
\]
\[
= \det \left[ λ^2 I_n - \text{Im} F(N^T) \text{Im} F(N) \right] = P(-λ),
\]
which shows that the Fourier transformation (11) does not converge for the symbols (E-9) and in (E-10), exactly as in previous example. Despite of these, the PF can be calculated, since the Weyl symbol (E-9) is well defined, which gives, for \( ν_{S_β} = 0 \),
\[
Z_β = \frac{1}{2^n} \csc \left( \frac{\hbar κβ}{2} \right)^n,
\]
which is the PF of \( n \) non-interacting unidimensional systems described by (E-11).

For illustration, consider the case \( n = 2 \). The Hamiltonian is \( H(x) = κ(p_1 q_1 + p_2 q_2 - p_1 q_2) \) and the Hessian (E-13) becomes
\[
H = \begin{pmatrix}
0_2 & \mathbf{K} \\
\mathbf{K}^T & 0_2
\end{pmatrix}, \quad \mathbf{K} := \begin{pmatrix}
κ & 0 \\
-κ & κ
\end{pmatrix}.
\]

The complex symplectic matrix in (E-14) is
\[
S_β = \begin{pmatrix}
1 & 0 \\
iβ & 1
\end{pmatrix} e^{-iβ}, \quad \begin{pmatrix}
1 & -iβ \\
iβ & 1
\end{pmatrix} e^{iβ}, \quad β := \hbar κβ,
\]
and the Cayley parametrization (E-15) is written with
\[
F(N) = i \begin{pmatrix}
\tan\left(\frac{\beta}{2}\right) & 0 \\
\frac{\beta}{2} \csc^2\left(\frac{\beta}{2}\right) & \tan\left(\frac{\beta}{2}\right)
\end{pmatrix},
\]
from where the four eigenvalues of \(\text{Im} \ C_{\beta} \) are obtained,

\[
\text{Spec}(\text{Im} \ C_{\beta}) = \left\{ \pm \bar{\beta} \pm \sqrt{\bar{\beta}^2 + 4 \sin^2 \beta} \over 2 + 2 \cos \beta \right\},
\]
and constitutes pairs of symmetric values.

6.4. Elliptic Hamiltonian

The one degree of freedom harmonic oscillator is the textbook example for the Wick mapping and by this reason deserves attention in the picture presented here.

The Hessian of the Hamiltonian and the Hamiltonian matrix are, respectively, \(H = \omega l_2\) and \(JH = \omega J\). The complex symplectic matrix (28) becomes

\[
S_{\bar{\beta}} = \begin{pmatrix}
\cosh \bar{\beta} & -i \sinh \bar{\beta} \\
i \sinh \bar{\beta} & \cosh \bar{\beta}
\end{pmatrix}, \quad \bar{\beta} := \hbar \omega \beta;
\]
its Cayley parametrization (41) is

\[
C_{\bar{\beta}} = -i \tanh\left(\frac{\bar{\beta}}{2}\right) l_2,
\]
and

\[
\det(S_{\bar{\beta}} - l_{2n}) = -4 \sinh^2\left(\frac{\bar{\beta}}{2}\right),
\]
\[
\det(S_{\bar{\beta}} + l_{2n}) = 4 \cosh^2\left(\frac{\bar{\beta}}{2}\right).
\]

From the above determinants, the symbol \(\tilde{E}_{\beta}(\xi)\) is not defined only for \(\beta = 0\), while the limit (60) imposes \(\nu_{\beta}^\dagger = 0\) for the same value of \(\beta\). Also note that there are no other divergences for both symbols, in such a way that the symplectic Fourier transform (11) interchanges both representations at all with the indexes given by (61), since \(\text{Im} \ C_{\beta} < 0, \forall \beta > 0\).

The Weyl and Wigner symbols becomes, respectively,

\[
\tilde{E}_{\beta}(\xi) = \frac{\exp\left[ -\frac{1}{4} i \tgh\left(\frac{\bar{\beta}}{2}\right) \xi^2 \right]}{2 \sinh\left(\frac{\bar{\beta}}{2}\right)}, \quad \text{(E-16)}
\]
\[
E_{\beta}(x) = \frac{\exp\left[ -\frac{1}{4} i \tgh\left(\frac{\bar{\beta}}{2}\right) x^2 \right]}{2 \cosh\left(\frac{\bar{\beta}}{2}\right)}.
\]
and the PF (65) becomes

\[
Z_{\beta} = \frac{1}{2} \text{csch}\left(\frac{\bar{\beta}}{2}\right). \quad \text{(E-17)}
\]
The widely known ‘Williamson theorem’ [30] is strictly connected with the elliptic case. Let $M \in \text{Mat}(2n, \mathbb{R})$ be any symmetric positive definite matrix: $M = M^\top > 0$. The theorem states that this matrix can be diagonalized by a symplectic congruence, i.e., there exists $S_M \in \text{Sp}(2n, \mathbb{R})$ such that

$$S_M^\top M S_M = \Lambda_M \oplus \Lambda_M,$$

(E-18)

with $\mu_j > 0$. The diagonal matrix $\Lambda_M$ is called the **symplectic spectrum** of $M$ and $\mu_i$ the symplectic eigenvalues. These can be found to be the (euclidean) eigenvalues of $JM$, i.e.,

$$\text{Spec}_C(JM) = \text{Diag}(i\mu_1, \ldots, i\mu_n, -i\mu_1, \ldots, -i\mu_n).$$

(E-19)

Thus, any positive QH, i.e., one such that $H_{cl} = \frac{1}{2} x \cdot M x$ with $M > 0$, has the collection of harmonic oscillators, with frequencies given by the symplectic spectrum $\Lambda_M$, as a normal form. The covariance relations (63) will give the symbols relative to

$$H'_{cl} = H_{cl}(S_M x) = \frac{1}{2} x \cdot \Lambda_M x = \sum_{j=1}^n \frac{\mu_j}{2} (q_j^2 + p_j^2),$$

in terms of the product of $n$ symbols, one symbol in (E-16) for each frequency in $\Lambda_M$. Similarly, the PF will be product of $n$ PFs in (E-17). This is nothing but un-revealing the normal-modes of a system of interacting oscillators, examples can be found in [31].

By another side, it is possible to show that the spectrum of a Hamiltonian matrix $JM$ is equal to the one in (E-19) if and only if $M > 0$, see [35]. Consequently, all thermal states generated by the QH in (48), or the symplectic matrix in (28), are in category (E) with $H = M$, if and only if the Hessian of the QH is positive-definite, $M > 0$. In this case, using the covariance relation in (64) with $Q = S_M$, for $S_M$ in (E-18), one finds

$$S_M' = e^{-i \hbar \beta \Lambda_H} = \cosh \left( \frac{1}{2} \hbar \beta \Lambda_H \right) - i \sinh \left( \frac{1}{2} \hbar \beta \Lambda_H \right),$$

where the last equality is obtained by a Taylor expansion of the exponential and noting that $[\Lambda_H, J] = 0$. From equation (41), the Cayley parametrization for $S_M'$ reads

$$C_S' = -i \tgh \left( \frac{1}{2} \hbar \beta \Lambda_H \right).$$

The covariance relation in (53) enables one to find the Cayley parametrization for the original Hamiltonian, viz,

$$C_{S, \beta} = S_M^\top C_{S, \beta} S_M^{-1} = -i S_M^\top \tgh \left( \frac{1}{2} \hbar \beta \Lambda_H \right) S_M^{-1}.$$

Since $\tgh(\frac{1}{2} \hbar \beta \Lambda_H) > 0$ for $\beta > 0$, equation (54) shows that $\text{Im} C_{S, \beta} < 0$, and the symbols for the thermal operator in equations (57), (58) or the functions in (62) are all Gaussians.

Using the Williamson theorem for the matrix $\Lambda_H' = \tgh(\frac{1}{2} \hbar \beta \Lambda_H)$, the matrix $\text{Im} C_{S, \beta}$ (for above $C_{S, \beta}$) is able to produce any symmetric positive-definite matrix. In such a way, all Gaussian states can be reproduced by equation (62) with above $C_{S, \beta}$. This also includes the pure states as the limit $\beta \to \infty$. 

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6.5. Loxodromic Hamiltonian

The loxodromic case can occur only in a phase space with at least four dimensions, what can be seen by the quartet structure of the eigenvalues in (L). Examples of systems where it appears are the ones in which a body subjected to an attractive potential also experiences torque forces, for instance, a spherical pendulum in which the symmetry axis itself is rotating with constant zenithal angular velocity [7]. In these systems, centrifugal (centripetal) resultants push (pull) the body away from (toward) an equilibrium configuration, which acting together with the attractive force, cause spiraling movements in phase space, see equation (E-20).

The Hamiltonian normal form of a system with two degrees of freedom in category (L) is [23]

\[
H_{\text{cl}} = \kappa (p_1 q_1 + p_2 q_2) + \omega (p_2 q_1 - p_1 q_2).
\]

The Hessian and the corresponding Hamiltonian matrix are

\[
H = \begin{pmatrix} 0 & \Omega \\ \Omega^T & 0 \end{pmatrix}, \quad JH = \Omega^\top \oplus (-\Omega), \quad \Omega := \begin{pmatrix} \kappa & -\omega \\ \omega & \kappa \end{pmatrix},
\]

which generates the symplectic matrix

\[
S_t = R_t e^{\omega t} \oplus R_t e^{-\omega t} \in \text{Sp}(4, \mathbb{R}), \quad (E-20)
\]

with

\[
R_t := \begin{pmatrix} \cos(\omega t) & \sin(\omega t) \\ -\sin(\omega t) & \cos(\omega t) \end{pmatrix} \in \text{Sp}(2, \mathbb{R}).
\]

The complex symplectic matrix in (28) becomes

\[
S_\beta = R_\beta e^{-i\hbar \kappa \beta t} \oplus R_\beta e^{i\hbar \kappa \beta t},
\]

with

\[
R_\beta := \begin{pmatrix} \cosh(h\omega \beta) & -i \sinh(h\omega \beta) \\ i \sinh(h\omega \beta) & \cosh(h\omega \beta) \end{pmatrix}.
\]

The Cayley parametrization is

\[
C_{\beta} = -i \begin{pmatrix} 0 & S \\ S^\top & 0 \end{pmatrix}.
\]
with

\[ S := \frac{\begin{pmatrix} \sin(\kappa \beta \hbar) & - \sinh(\hbar \omega \beta) \\ \sinh(\hbar \omega \beta) & \sin(\kappa \beta \hbar) \end{pmatrix}}{\cosh(\hbar \omega \beta) + \cos(\hbar \kappa \beta)} \]

and the four eigenvalues of \( \text{Im } C_{S_\beta} \) are

\[ \text{Spec}(\text{Im } C_{S_\beta}) = \left\{ \pm \sqrt{\cosh(2\hbar \omega \beta) \pm \cos(2\hbar \kappa \beta)} \right\}, \]

which are pairs of symmetric real numbers. Since

\[ \det(S_\beta \pm \lambda) = 4[\cos(\hbar \kappa \beta) \mp \cosh(\hbar \omega \beta)]^2, \]

there is no Weyl representation only for \( \beta = 0 \), while the Wigner representation is well defined for any value \( \beta \geq 0 \). However, since the eigenvalues of \( \text{Im } C_{S_\beta} \) have different signs, these symbols are not related by the Fourier transformation (11). From (60), and since there are no divergences, \( \nu^+_\beta = 0, \forall \beta > 0 \), and also \( \nu^-_\beta = 0 \), due to the positivity of the PF in (65).

The PF in (65) becomes

\[ Z_{\beta} = \frac{1}{2}[\cosh(\hbar \omega \beta) - \cos(\hbar \kappa \beta)]^{-1}, \]

and the heat capacity in (69),

\[ C = k_B \hbar^2 (\omega^2 - \kappa^2) \beta^2 \frac{\cosh(\beta \omega \hbar) \cos(\beta \kappa \hbar) - 1}{[\cos(\beta \kappa \hbar) - \cosh(\beta \omega \hbar)]^2}
+ 2 k_B \hbar^2 \kappa \omega \beta^2 \frac{\sinh(\beta \omega \hbar) \sin(\beta \kappa \hbar)}{[\cos(\beta \kappa \hbar) - \cosh(\beta \omega \hbar)]^2}. \]

Both are plotted in figure 2 and from there it is possible to observe that the parameter \( \kappa \) controls the oscillatory behavior, while \( \omega \) controls the amplitude. In agreement with (71), \( \lim_{\beta \to 0} C = 2k_B \). The thermodynamical instability of this kind of systems, associated to negative values of the heat capacity [1], is a property of the whole class (\( L \)), since the heat capacity is related to the concavity of the PF, see equation (69), and the PF only depends on the eigenvalues of the Hamiltonian matrix \( J_H \).

7. Conclusions

The class of Hamiltonian systems is extensively broader than the quadratic case, notwithstanding, as it is learnt from dynamical systems, much of the system evolution is grasped on its fixed points whose nature determines locally the system behavior through a linearization, rising a QH. Under this perspective, it is opportune to conclude with some remarks on missing points and possible extensions.

The prototype of a thermodynamical system is the ideal gas [1], which is a system described by a QH in class (\( P \)) and with Hessian as that one in (E-3). As a mechanical system, a canonical transformation of phase space coordinates would not change its physical properties. Nevertheless, its PF (E-6) and all of its thermodynamical properties definitively are not subjected to the covariance rules in section 3.4. Technically speaking, this is due to the performed truncation of an integral in (E-6). Physically, the reason relies on the imposition of a container with finite
volume, which appears as a ‘contour-condition’, or a non-holonomic constraint, whence not canonically covariant.

The divergences of the PF for the Hamiltonian systems in category (H) are not tamed by such kind of constrain, see equation (E-12), showing that these are related to distinct properties of a thermodynamical system. At this point, the advantages of the Wigner–Weyl representations become clear: the analytical expression of the PF is obtained through the Weyl representation, despite the non-convergence of the integral of the Wigner symbol (E-10). Such kind of divergence, a consequence of the sum in the PF for a continuous and unbound energy levels of the hyperbolic Hamiltonian [36], is what happens in scattering problems, which is exemplified at the end of section 6.2.

A diverging (or not converging) PF in principle is a pathology for the statistical treatment of physical systems. Quoting Gibbs [37], ‘we shall always suppose the (…) [PF] to have a finite value, as otherwise the coefficient of probability vanishes, and the law of distribution becomes illusory. This will exclude certain cases (…) for instance, cases in which the system or parts of it can be distributed in unlimited space (…)’. If, by one side, the non-convergence for the category (P) is amended by the constrain imposition, category (H) [and also (L)], as it is, can play a privileged role in the development of a full dynamical background to statistical physics, since these Hamiltonians are the ones which possesses positive Lyapunov exponents, which are responsible for the phenomena of mixing in classical chaotic Hamiltonians [8, 10]. The relation of mixing and relaxation to equilibrium is a question posed in [38] and analyzed for chaotic billiards. It remains an open question for generic non-linear Hamiltonians.

The other prescription of exclusion in [37] is when ‘the energy can decrease without limit, as when the system contains material points which attract one another inversely as the squares of their distances’. While classically, it is impossible to write a PF for gravitational or Coulomb interacting particles due to the boundlessness of system energy, the quantum PF of such systems also diverges, but due to the energy level spacing structure [39]. Despite such Hamiltonians does not have any fixed point, since they are such that $\partial H/\partial x \neq 0$, the dynamics of the radial coordinate [23] lives in a bifurcative scenario between (E) and (H): negative energies originate ellipses, zero energy trajectories are parabolas, and positive energy are hyperbolas in configuration space. This bifurcative behavior and its relation with the divergence of PF, both classical and quantum, should be clarified in a future work.

From the case of (H), the thermal capacity diverges when the temperature approaches zero, which is also a consequence of the boundlessness of the system, since at this temperature limit it does not attain a ground state, a prerequisite of the Nernst principle [1]. More interesting is the category (L), where the system has negative heat capacity for certain ranges of temperatures, see figure 2. However, be in this category is only a sufficient condition for a system to present this behavior. The system presented in [40] is a collection of two dimensional rotors (four dimensional phase-space). The Hamiltonian of two interacting rotors has a fixed point associated simultaneously with a pair of eigenvalues in (P) and another pair in (E). This seems to show that a combination of different categories can generate the negative specific heat, which is out of the scope of this work, however should be investigated. Another example where there is a combination of categories for the same fixed point is [41] and again the system has a negative heat capacity. Both systems in [40, 41] have long-range interactions and one can not expect that the local approximation developed in section 5 to work. A better method of approximation which takes into account the influence of multiple or hybrid fixed points spread in phase space should be developed.

Few months after the submission of this work, the reference [42] dealing with similar questions have appeared in arXiv.
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