Williamson theorem in classical, quantum, and statistical physics

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In this work we present (and encourage the use of) the Williamson theorem and its consequences in several contexts in physics. We demonstrate this theorem using only basic concepts of linear algebra and symplectic matrices. As an immediate application in the context of small oscillations, we show that applying this theorem reveals the normal-mode coordinates and frequencies of the system in the Hamiltonian scenario. A modest introduction of the symplectic formalism in quantum mechanics is presented, using the theorem to study quantum normal modes and canonical distributions of thermodynamically stable systems described by quadratic Hamiltonians. As a last example, a more advanced topic concerning uncertainty relations is developed to show once more its utility in a distinct and modern perspective.

I. INTRODUCTION

The main advantage of the Hamiltonian formalism in classical mechanics is the symmetry of the equations of motion with respect to position and momentum coordinates, which naturally embody the symplectic structure of the phase space. The same structure is also present in quantum mechanics through position and momentum operators of the systems, which in either classical or quantum physics is the arena for the Williamson theorem that describes a diagonalization procedure suitable to the symplectic scenario. Just as diagonalizing a matrix in Euclidean space determines invariant quantities (eigenvalues and eigenvectors), applying the Williamson theorem reveals various properties of symplectic invariance.

The initial part of this paper, Section II, introduces the mathematical notation and then presents the Williamson theorem, which is proved in the Supplementary Material using only basic concepts in linear algebra.

The central application is the study of small oscillations in the context of Hamiltonian dynamics, which is performed by the diagonalization of a positive-definite form through the use of the theorem. To present this study, Sec.III reviews Hamiltonian mechanics and then treats quadratic Hamiltonians using the theorem. The standard method of dealing with the problem of small oscillations (the simultaneous diagonalization of the kinetic and potential terms of a Lagrangian function) is compared with the Hamiltonian results in the Supplementary Material. The advantages of the Williamson theorem become clear in this context: a change of coordinates in phase space reveals the normal modes and the eigenfrequencies of the system.

In Section IV, initial concepts of the symplectic formalism in quantum mechanics are described that allow the theorem to be used to study small oscillations in quantum systems. Because creation-annihilation operators are often used in study of oscillations, these operators are placed in a (complex) symplectic scenario, suitable to the application of the theorem.

The previous applications lead immediately to the use of the theorem to study the canonical equilibrium ensemble of statistical physics. In Section V, the equilibrium state and the partition function associated with a generic quadratic Hamiltonian are determined for thermodynamically stable systems, where the normal-mode frequencies play the fundamental role, showing that all the thermodynamical properties of the system are symplectically invariant.

Crossing the frontier towards modern research, Section VI contains a pedagogical derivation for the Robertson-Schrödinger uncertainty relation, which is a generalization of the Heisenberg principle. The application of the theorem reveals invariant properties common to all physical states. This content is inspired by the results in Ref.15, probably the first paper in physics introducing the theorem in the sense presented here.

Section VII concludes by presenting comments on generalizations of the theorem and references to modern applications. The idea behind this manuscript is to bring it to classroom, showing how standard problems in physics courses can be treated using this simple and unified perspective.

Physically motivated examples are presented in the Supplementary Material.

A starting example:

Consider a system with one degree of freedom described by the Hamiltonian

$$H(q, p) = \frac{a}{4}(q/q_0 + p/p_0)^2 + \frac{b}{4}(q/q_0 - p/p_0)^2, \quad (1)$$

where \(q\) is the generalized coordinate; \(p\) the canonically conjugated momentum; and \(a, b, q_0, \) and \(p_0\) are real constants. Without loss of generality, one can choose \(q_0 p_0 = 1,\) which is nothing but a choice of units. If

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for $x$, symplectic diagonalization forms a matrix $S$ which is such that

\[
S \text{ is symplectic and that the symplectic eigenvalue is equal to state that every } x \text{ or } S \text{ is a symplectic matrix with a symplectic eigenvalue.}
\]

These concepts will be defined soon; for now it is enough to state that every $2 \times 2$ real matrix with unity determinant is symplectic and that the symplectic eigenvalue is not equal to an ordinary (Euclidean) eigenvalue.

The relation between the Hamiltonian and matrix $S$ is established when considering the Hessian

\[
H := \begin{pmatrix} \frac{\partial^2 H}{\partial x \partial \dot{x}} & \frac{\partial^2 H}{\partial p \partial \dot{p}} \\ \frac{\partial^2 H}{\partial x \partial p} & \frac{\partial^2 H}{\partial p \partial p} \end{pmatrix} = \begin{pmatrix} a + b & \frac{a - b}{2} \\ \frac{2a'}{q_0^2} & a + b \end{pmatrix},
\]

which is such that $S^T H S = \text{Diag}(\sqrt{ab}, \sqrt{ab}) =: \mathbf{H}'$, where $S^T$ is the transpose of $S$. Here the matrix $S$ performs a symplectic diagonalization of $H$, which is not a coincidence, but rather a consequence of the symplectic structure of phase space manifested through the identity

\[
A = JH, \text{ where } J := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.
\]

Noteworthy: $A' = JH'$, where $H'$ is the Hessian of $H'(q', p')$.

Diagonalizing the matrix $A$ reveals that its eigenvalues are $\pm i\sqrt{ab}$, which are complex if $ab > 0$. The equations of motion could be decoupled using the (complex) coordinates $w := Bx$, where $A' = BAB^{-1}$ is diagonal. However, all the phase-space properties would be lost; for instance, it would be impossible to attain a real Hamiltonian function for the decoupled degrees of freedom. The great advantage of the symplectic change of coordinates is that it rewrites the dynamics of the original system as a mechanically equivalent system, preserving all the structure and symmetry of phase space.

The Lagrangian function for the same system is obtained by the Legendre transformation for the original Hamiltonian,

\[
L(q, \dot{q}) = p(q, \dot{q}) - H(q, p(q, \dot{q})) = \frac{(q - aq)(\dot{q} + bq)}{(a + b)q_0^2},
\]

where the function $p(q, \dot{q})$ was obtained from equation $\dot{q} = \partial H/\partial p$ to be $p = (2q + (b - a)\dot{q})/[(a + b)q_0^2]$. Using the Euler-Lagrange equation, the generalized coordinate satisfies $\dot{q} + (ab) q = 0$, which is the same requirement as obtained for $q'$ in the Hamiltonian scenario. Up to this point, the Lagrangian treatment seems to be simpler and straightforward.

However, the Heisenberg equations for the dynamics governed by the quantization of the original Hamiltonian,

\[
\hat{H} := H(\hat{q}, \hat{p}) = \frac{a}{4}(\hat{q}/q_0 + \hat{p}/p_0)^2 + \frac{b}{4}(\hat{q}/q_0 - \hat{p}/p_0)^2,
\]

are given by

\[
\frac{d\hat{q}}{dt} = \frac{i}{4}[\hat{H}, \hat{q}] = \frac{i}{2}(a - b)\hat{q} + \frac{i}{2}(a + b)\hat{p}/p_0^2,
\]

\[
\frac{d\hat{p}}{dt} = \frac{i}{4}[\hat{H}, \hat{p}] = -\frac{i}{2}(a + b)\hat{q}/q_0^2 + \frac{i}{2}(b - a)\hat{p},
\]

which are the same as the classical ones if one replaces $q \rightarrow \hat{q}$ and $p \rightarrow \hat{p}$. It is thus possible to apply the same linear canonical transformation at the operator level, attaining the equivalence with a Hamiltonian system of quantum oscillators under the same condition $ab > 0$. This compatibility of classical and quantum scenarios clearly constitutes a huge advantage over the Lagrangian description.

An immediate but not obvious question is to what extent the above symplectic procedure can be applied to more complex (classical or quantum) systems. The answer will be given by the Williamson theorem, which will provide conditions for a Hamiltonian system to behave like a set of harmonic oscillators.

Another introductory example can be found in Supplementary Material, where the Lagrangian treatment of small oscillations is performed and compared with the symplectic diagonalization scheme for a physical interfering problem, namely, the dynamics of two interacting trapped ions.
II. WILLIAMSON THEOREM

The question addressed by the Williamson theorem is the diagonalization of positive definite matrices through symplectic matrices. Before the presentation of the theorem, some basic concepts concerning these kinds of matrices and some linear algebra will be reviewed.

A vector \(v \in \mathbb{R}^n\) is a column of \(n\) real components \(v_i\), with \(i = 1, ..., n\) and its transposition is the line vector \(v^\top := (v_1, ..., v_n)\). The scalar product between \(u, v \in \mathbb{R}^n\) is defined by \(u \cdot v := u^\top v = \sum_{i=1}^{n} u_i v_i \in \mathbb{R}\). For two complex vectors \(z, w \in \mathbb{C}^n\), their scalar product is \(z^\dagger w := \sum_{i=1}^{n} z_i^* w_i \in \mathbb{C}\), where \(z^\dagger := (z_1^*, ..., z_n^*)\). The set of all \(n \times n\) complex square matrices is denoted by \(M(n)\), and for real matrices the notation \(M(n, \mathbb{R})\) will be used. Note that \(M(n, \mathbb{R}) \subset M(n)\). The identity and null matrices in \(M(n)\) are respectively denoted by \(I_n\) and \(0_n\).

Two matrices \(A, B \in M(n)\) are said similar, if there exists an invertible \(C \in M(n)\) such that \(A = CBC^{-1}\). This relation corresponds to a change of basis in linear algebra, i.e., \(w = Bz\) is equivalent to \(Cw = Az\), for \(z \in \mathbb{C}^n\). From this point of view, a similarity is related to structures of the transformation that are common to any basis of the space. The matrices \(A\) and \(B\) in this case share the same spectrum; that is, they have the same eigenvalues, since \(\det(A - \lambda I_n) = \det(B - \lambda I_n)\).

In this perspective, eigenvalues are invariant under a similarity relation, while eigenvectors are covariant; that is, if \(z\) is an eigenvector of \(B\), then \(Cz\) is an eigenvector of \(A\). A diagonalizable matrix is the one that is similar to a diagonal matrix and the spectral theorem\(^\text{18}\) sets a necessary and sufficient condition for it: a matrix \(A \in M(n)\) is normal (i.e., \(A^\dagger A = AA^\dagger\)) if and only if it is unitarily similar to a diagonal matrix, which contains the eigenvalues of \(A\). For the similarity relation above, this means that \(A\) is normal if and only if there is a \(C\) satisfying \(C^\dagger C = C^{-1}\) such that \(B\) is diagonal.

Unitary matrices, which include either complex or real orthogonal matrices, are isometries of the Euclidean space, which means that they preserve the scalar product (or the “distance”): \(w_1^\dagger z = (Uw_1)^\dagger Uz\), since \(U^\dagger U = I_n\), for \(U \in M(n)\) and \(w, z \in \mathbb{C}^n\). Whenever a diagonalization of a matrix is performed through either an orthogonal or a unitary similarity relation, which is the common sense for a diagonalization (through the spectral theorem), it will be called an Euclidean diagonalization and the eigenvalues as the Euclidean eigenvalues. This nomenclature emphasizes the difference from another kind of diagonalization performed in the Williamson theorem, which will be a symplectic diagonalization.

A weaker relation than similarity, but no less important here, is called congruence. Two matrices \(A, B \in M(n)\) are said to be congruent if there exists a invertible \(C \in M(n)\) such that \(A = CBC^\dagger\). Now, neither the spectrum nor the eigenvectors play a privileged role; however the inertia\(^\text{19}\) of \(A\) and \(B\) will be the same if and only if these matrices are Hermitian. This invariance property is known as Sylvester’s law of Inertia\(^\text{20}\), a kind of “spectral theorem” for congruence relations. When matrix \(C\) is unitary or orthogonal, the congruence \(A = CBC^\dagger\) is also a similarity.

A matrix \(A \in M(n)\) is said positive-definite, denoted by \(A > 0\), if \(w^\dagger Aw > 0\), \(\forall w \in \mathbb{C}^n\); if \(A\) is Hermitian, \(A = A^\dagger\), the last statement is equivalent to saying that all eigenvalues of \(A\) are real and positive\(^\text{18}\). Consequently, all Hermitian positive-definite matrices are invertible, since \(\det A > 0\). For \(A^\dagger = A > 0\), the unique matrix \(\sqrt{A} \in M(n)\) satisfying

\[
(\sqrt{A})^2 = A \quad \text{and} \quad \sqrt{A}^\dagger = \sqrt{A} > 0 \quad (11)
\]

is the positive square-root\(^\text{18}\) of \(A\). If the eigenvalues of a Hermitian matrix \(A \in M(n)\) are non-negative (they can be either positive or zero), the matrix is positive semi-definite (denoted by \(A \geq 0\)) and is equivalent to \(w^\dagger Aw \geq 0\), \(\forall w \neq 0\). A trivial corollary of the Sylvester law relates positivity and congruences: Let \(A, B, C \in M(n)\), such that \(A = CBC^\dagger\) with \(\det C \neq 0\); for \(w \in \mathbb{C}^n\), \(w^\dagger Aw = (Cw)^\dagger BC^\dagger w\), thus \(A \geq 0\) (resp. \(A > 0\)) if and only if \(B \geq 0\) (resp. \(B > 0\)).

A matrix \(M \in M(2n)\) can be written as a block matrix when portioned by smaller matrices\(^\text{18}\):

\[
M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad A, B, C, D \in M(n), \quad (12)
\]

where \(A_{ij} = M_{ij}\) for \(i, j \leq n\), \(B_{ij} = M_{ij}\) for \(i \leq n \land n + 1 \leq j \leq 2n\), etc. As a compact and useful notation, the direct sum\(^\text{18}\) \(A \oplus D\) is a block-diagonal matrix, i.e., the above matrix \(M\) with \(B = C = 0_n\). The determinant of a block matrix can be expressed in terms of its blocks\(^\text{18, 21}\), for instance, \(\det M = \det D \det (A - BD^{-1}C)\), if \(D\) is nonsingular. If in addition \([C, D] = 0\), then \(\det M = \det (AD - BC)\). All the above properties and formulas can be generalized for nonsquare blocks, different partitions, or even singular blocks\(^\text{18}\).

A symplectic matrix \(S \in M(2n, \mathbb{R})\) is defined by the rule

\[
S^\top JS = J, \quad \text{where} \quad J = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix} \in M(2n, \mathbb{R}). \quad (13)
\]

The matrix \(J\) is such that \(J^2 = -I_{2n}\), thus \(J^{-1} = -J = J^\top\), and is itself a symplectic matrix with \(\det J = 1\). Taking the transposition of \(S\), one shows that \(S^\top\) is also symplectic and that the condition \(SJS^\top = J\) is equivalent to Eq. (13). The determinant of a symplectic matrix, from the definition, is such that \(\det S^2 = 1\). Consequently, every symplectic matrix is invertible and the inverse is \(S^{-1} = J^\top S^\top J\) by Eq. (13). Finally, the set of symplectic matrices forms the group

\[
\text{Sp}(2n, \mathbb{R}) := \{ S \in M(2n, \mathbb{R}) \mid S^\top JS = J \}, \quad (14)
\]

since \(I_{2n} \in \text{Sp}(2n, \mathbb{R})\), \(S^{-1} \in \text{Sp}(2n, \mathbb{R})\) if \(S \in \text{Sp}(2n, \mathbb{R})\), and \(S_1 S_2 \in \text{Sp}(2n, \mathbb{R})\) if \(S_1, S_2 \in \text{Sp}(2n, \mathbb{R})\). It is not difficult to show that condition Eq. (13) reduces to \(\det S = 1\) for \(n = 1\); in other words, every \(2 \times 2\) real matrix with
determinant one is a symplectic matrix. Every matrix $S \in \text{Sp}(2n, \mathbb{R})$ has determinant one; however, this fact does not have a simple proof\(^{22}\). Although (13) seems related to $O^\top I_n O = I_n$, symplectic matrices are in general not isometries since $S^\top S \neq I_{2n}$. However, a symplectic isometry does exist for the particular case where symplectic matrices are also orthogonal\(^5,6\). It is important to keep in mind that the symplectic group in this work is defined only for even-dimensional real matrices; that is, matrices in $M(2n, \mathbb{R})$.

In this paper all symplectic matrices, excepting the identity $I_{2n}$, will be typed with sans-serif fonts, e.g., $J, S, Z, O, L$, etc, while all the other matrices appear as Roman bold.

For each real square positive-definite symmetric matrix with even dimension, there is an associated symplectic matrix that diagonalizes it through a congruence relation in a very specific way. This is the content of the Williamson theorem\(^5,15,23\).

**Theorem:** Let $M \in M(2n, \mathbb{R})$ be symmetric and positive-definite, i.e., $M^\top = M > 0$. There exists $S_M \in \text{Sp}(2n, \mathbb{R})$ such that

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

with $0 < \mu_j \leq \mu_k$ for $j \leq k$. Each $\mu_j$ is such that

$$\det(JM \pm i \mu_j I_{2n}) = 0 \quad (j = 1, ..., n),$$

and the matrix $S_M$ admits the decomposition

$$S_M = \sqrt{\Lambda_M} O \sqrt{M^{-1}},$$

where $O \in M(2n, \mathbb{R})$ satisfies

$$O \sqrt{M} J \sqrt{M} O^\top = \Lambda_M J,$$

and $O^\top = O^{-1}$, i.e., is an orthogonal matrix.

Before going into the proof, some comments are in order: — The matrix $S_M$ performs a symplectic diagonalization through a congruence relation between $M$ and $\Lambda_M$, although generic congruences are not similarity relations. — The double-paired ordered set (or the diagonal matrix) $\Lambda_M \in M(2n, \mathbb{R})$ is called symplectic spectrum of $M$ and $\mu_k$ are said to be its symplectic eigenvalues, which are in general not equal to a Euclidean eigenvalue of $M$. In addition $S_M = S_M^{-1}$, that is, $S_M$ is symplectic and orthogonal, the matrix $M$ will be orthogonally similar to $\Lambda_M$. In this situation the symplectic and Euclidean spectrum coincide.

— The complex numbers $\pm i \mu_j$, where $\mu_j > 0$, $\forall j$, are the Euclidean eigenvalues of $J M$.

— The symplectic congruence $M' := S^\top M S$ for any $S \in \text{Sp}(2n, \mathbb{R})$ is equivalent to the similarity $J M' = S^{-1} J M S$, due to the symplectic condition for $S$. Explicitly, $J S^\top M S = S^{-1} J M S$.

— The symplectic spectrum is invariant under symplectic congruences, which means that for any $S \in \text{Sp}(2n, \mathbb{R})$, the symplectic spectrum $\Lambda_{M'}$ of $M' := S^\top M S$ is also $\Lambda_M$ owing to the similarity $J M' = S^{-1} J M S$.

— Due to $\det S_M = \det I = 1$, then $\det M = \det \Lambda_M = \det J M = \mu_1^2 \mu_2^2 \cdots \mu_n^2$. If $n = 1$, $\Lambda_M = \mu_1 I_2$ and $\det M = \mu_1^2$.

— The matrix Eq. (17) readily satisfies $S_M M S_M^\top = \Lambda_M$ for any orthogonal matrix $O$; however $S_M$ in Eq. (17) will be symplectic if and only if the orthogonal matrix obeys Eq. (18).

— There are several situations in physics where only the symplectic spectrum of a positive-definite matrix $M$ is required; following Eq. (13), this spectrum is directly obtained through the solution of $\det(JM - \mu I_{2n}) = 0$, i.e., from the Euclidean eigenvalues of $JM$.

— The matrix $S_M$ can be constructed after the determination of the symplectic spectrum. To this end, the matrix $M$ must be Euclideanally diagonalized and its square root determined. To obtain the orthogonal matrix $O$, the system of equations in Eq. (18), which has a unique solution for $O$, must be solved, and thus Eq. (17) provides the desired symplectic matrix.

— Squaring both sides of Eq. (18) results in $-A_M^2 = O(\sqrt{M} J \sqrt{M} O^\top)$, which shows that the symmetric matrix in the parentheses is Euclideanally diagonalized by the matrix $O$. The solution of the above eigensystem is in general more convenient than solving Eq. (18).

A detailed proof of the theorem, thought to be pedagogical and self-contained, is placed in the Supplementary Material; nevertheless an outline (based on Ref.23) may be valuable at this stage.

**Outline of the Proof:** The main point relies upon the Euclidean diagonalization of skew-symmetric matrices, in particular the corollary for an even-dimensional nonsingular skew-symmetric matrix\(^{24}\): the matrix $M \in M(2n, \mathbb{R})$ is invertible and skew-symmetric, $M^\top = -M$, if and only if there is an orthogonal matrix $Q \in M(2n, \mathbb{R})$ such that $Q M Q^\top = J(\Omega \oplus \Omega)$, where $J$ is defined in Eq. (13) and $\Omega = \text{Diag}(\omega_1, ..., \omega_n)$ with $\omega_j > 0$, $\forall j$.

The eigenvalues of $M$ are the roots of $\det(M - \lambda I_{2n}) = \det[J(\Omega \oplus \Omega) - \lambda I_{2n}] = 0$; this last determinant may be evaluated through blocks, i.e., $\det[J(\Omega \oplus \Omega) - \lambda I_{2n}] = \det(-\lambda \Omega, \Omega_{-\lambda}) = \det(\Omega^2 + \lambda^2 I_n) = 0$, and thus the eigenvalues are $\pm i \omega_j$, for $j = 1, ..., n$.

The matrix in Eq. (17) is the most generic matrix satisfying Eq. (15), since $O$ is a generic orthogonal matrix; writing $M := \sqrt{M} J \sqrt{M}$, then $M = -M^\top$, since $M = M^\top$ and $J^\top = -J$. Consequently, $\det(M - \lambda I_{2n}) = \det(JM - \lambda I_{2n})$ and the eigenvalues of $JM$ will be as the ones above, which is expressed as Eq. (16).

Noting that $\det M = \det M > 0$, the above corollary is employed and it is possible to identify $(\Omega \oplus \Omega) = \Lambda_M$, and $Q = O$, thus $Q M Q^\top = J(\Omega \oplus \Omega)$ becomes exactly Eq. (18). Manipulating this last equation, one finds $J = (\sqrt{M})^{-1}(\Lambda_M J \sqrt{\Lambda_M})(\sqrt{M} O^\top)^{-1}$, which is a symplectic condition for the matrix $S_M$ in Eq. (17).
In the Supplementary Material, the proof is more detailed and does not assume a priori knowledge of the diagonalization properties of skew-symmetric matrices.

III. HAMILTONIAN DYNAMICS

The movement of a system in phase space is governed by the Hamilton equations

$$\dot{x} = \frac{dx}{dt} = J \frac{\partial h}{\partial x},$$

where $x := (q_1, ..., q_n, p_1, ..., p_n)^\top$ is the vector containing the generalized coordinates and momenta of the system, $J$ is the symplectic matrix in Eq. (13), and $h = H(x, t)$ is the Hamiltonian of the system.

A change of variables $x' = f(x, t)$ is said to be canonical if it preserves the equations of motion. This will happen if and only if the Jacobian matrix of the transformation $\partial f / \partial x \in M(2n, \mathbb{R})$ is a symplectic matrix (14); that is, if it satisfies Eq. (13). A canonical transformation is linear when the function $f$ is itself the linear function $f(x, t) = Sx$, for any symplectic $S$.

As an example (14), the one-degree-of-freedom polar (action-angle) transformation

$$f(x, t) = (\sqrt{2q} \cos p, \sqrt{2q} \sin p)$$

is canonical since the Jacobian matrix

$$\frac{\partial f}{\partial x} = \begin{pmatrix} \frac{1}{\sqrt{2q}} \cos p & \frac{1}{\sqrt{2q}} \sin p \\ \frac{1}{\sqrt{2q}} \sin p & \frac{1}{\sqrt{2q}} \cos p \end{pmatrix}$$

is symplectic thanks to $|\partial f / \partial x| = 1$; however $f$ is not linear.

For the remainder of this paper, only affine canonical transformations will be relevant. These are compositions of symplectic transformations with rigid translations:

$$f(x, t) = Sx + \eta,$$

for a symplectic $S$ and a $\eta \in \mathbb{R}^{2n}$; note that $\partial f / \partial x = S$.

The Poisson bracket between two functions $f(x, t)$ and $g(x, t)$ is written as

$$\{f, g\} := \frac{\partial f}{\partial x} \cdot \frac{\partial g}{\partial x};$$

the presence of the matrix $J$ indicates, and it is not difficult to show, that this structure is invariant under canonical transformations (14). Choosing $f(x) = x_j$ and $g(x) = x_k$, the fundamental Poisson bracket is obtained

$$\{x_j, x_k\} = J_{jk}.$$  

(24)

It is instructive and useful for the next section to show the invariance of Eq. (24) under affine symplectic transformations. Defining $x' := Sx + \eta$, then

$$\{x'_j, x'_k\} = \sum_{l,m=1}^{2n} S_{jl}S_{km}\{x_l, x_m\}$$

$$= (SJS^\top)_{jk} = J_{jk},$$

(25)

due to the symplectic nature of $S$.

A. Quadratic Hamiltonians and Williamson Theorem

Consider the time-independent quadratic Hamiltonian

$$H(x) = \frac{1}{2} x \cdot H x + x \cdot \xi + H_0,$$

(26)

where $\xi \in \mathbb{R}^{2n}$ is a vector, $H_0 \in \mathbb{R}$ is a constant, and $H = H^\top = \partial^2 H / \partial x \partial x$ is the Hessian matrix. The corresponding equations of motion follow immediately from Eq. (19) and using that $\partial H / \partial x = H x + \xi$, yielding

$$\dot{x} = JHx + J\xi.$$  

(27)

If $\det H \neq 0$, a direct substitution shows that the solution of Eq. (27) is given by

$$x(t) = S_t (x_0 + H^{-1} \xi) - H^{-1} \xi, \quad S_t := \exp [tJH]$$

(28)

for an initial condition $x_0 := x(0)$. The phase-space point $x_0 := -H^{-1} \xi$ is an equilibrium (or fixed) point of the system, since $x(t) = x_0, \forall t$, if $x_0 = x_\#$. Even when $\det H = 0$, an analytical solution like Eq. (28) can be obtained; see the Supplementary Material.

Due to the symmetricity of $H$, the above defined matrix $S_t$ is itself a symplectic matrix, since

$$JS_t J^{-1} = \exp [J^2 HJ^{-1} t] = \exp [-J(JH)^\top t]$$

$$= (\exp [-JHt])^\top = (S_t^{-1})^\top = (S_t^\top)^{-1},$$

(29)

where we used that $J^T = J^{-1} = -J$ and $\exp (A^\top) = (\exp A)^\top$; multiplying the above equation by $S_t^\top$ from the left and by $J$ from the right, the symplectic condition in Eq. (13) is obtained. Note also that $S_{-t} = S_t^{-1}$. It is noteworthy that the temporal evolution in Eq. (28) is an affine canonical transformation, as defined in Eq. (22).

All these properties remain valid for any matrix $H$; see the Supplementary Material.

Regardless of the analytic solution for a generic quadratic Hamiltonian, the behavior of the system (or the matrix $S_t$) can be very awkward due to the exponential structure in Eq. (28), even considering $\det H \neq 0$. Fortunately, the Williamson theorem is useful to simplify the description of the system’s behavior when $H$ is positive-definite.

Considering $H > 0$, Eq. (15) can be applied,

$$S_HHS_H^\top = \Lambda_H,$$

(30)

and the Hamiltonian Eq. (26) becomes

$$H(x) = \frac{1}{2} x \cdot S_H^\top \Lambda_H S_H^\top x + x \cdot \xi + H_0$$

$$= \frac{1}{2} S_H^\top x \cdot \Lambda_H S_H^\top x + S_H^\top x \cdot S_H \xi + H_0,$$

(31)

where, for compactness, we introduced the notation $A^{-\top} := (A^\top)^{-1} = (A^{-1})^\top$. Through the theorem, any quadratic Hamiltonian with a positive-definite Hessian describes a collection of $n$ harmonic oscillators, since performing the canonical transformation $x' := S_H^\top x$, for $S_H$ in Eq. (17), the Hamiltonian of the system turns into

$$H'(x') := H(S_H^\top x') = \frac{1}{2} x' \cdot \Lambda_H x' + x' \cdot S_H \xi + H_0$$

$$= \frac{1}{2} (x' - x'\#) \cdot \Lambda_H (x' - x'\#) + H_0,$$

(32)
where \( H'_0 := H_0 - \frac{1}{2} x'_* \cdot A_H x'_* \) is an (constant) offset of the Hamiltonian, \( x'_* := S_H^{-1} x_* = -A_H^{-1} S_H \xi \) is the equilibrium coordinate (fixed point of \( H' \)), and, from Eq. (15), the quadratic form is

\[
\frac{1}{2} (x' - x'_*) \cdot A_H (x' - x'_*) = \sum_{k=1}^{n} \frac{\mu_k}{2} (p'_k - p'_{*k})^2 + \frac{\mu_k}{2} (q'_k - q'_{*k})^2. \tag{33}
\]

The most important consequence of the Williamson theorem is expressed in the linear canonical transformation \( x' = S_H^{-T} x \), which brings the system to its normal-mode phase-space coordinates and reveals the eigenfrequencies of the system to be the symplectic eigenvalues contained in \( A_H \). Writing the equations of motion for the normal modes, i.e., performing the transformation \( x' = S_H^{-T} x \) in Eq. (19), the Hamilton equation becomes

\[
\dot{x}' = J \frac{\partial h'}{\partial x'} = J A_H (x' - x'_*), \tag{34}
\]

for \( h' = H'(x') \) in Eq. (32), with solution given by

\[
x'(t) = S'(x_0' - x'_*) + x'_*, \quad S'_t := \exp[J A_H t]. \tag{35}
\]

Recalling that \( J^2 = -I_{2n} \), the evolution matrix can be cast into the form

\[
S'_t = \exp[J A_H t] = \cos(A_H t) + J \sin(A_H t), \tag{36}
\]

since

\[
\exp[J A_H t] = \sum_{k=0}^{\infty} \frac{[\cos(A_H t)]^{2k}}{(2k)!} + \frac{[\sin(A_H t)]^{2k+1}}{(2k+1)!} = \sum_{k=0}^{\infty} \left[ (-1)^k \frac{\cos(A_H t)^{2k}}{(2k)!} + (-1)^k \frac{\sin(A_H t)^{2k+1}}{(2k+1)!} \right]. \tag{37}
\]

The symplectic matrix \( S'_t \) is also orthogonal,

\[
S'_t^{-1} = S'_{-t} = \exp[-J A_H t] = \exp[A_H J^T t] = S'_t^T, \tag{38}
\]

and the evolution of the system in Eq. (35) is thus a rotation in phase space around the equilibrium point \( x'_* \), where each conjugate pair evolves as

\[
\left( \begin{array}{c} q'_k(t) - q'_{*k} \\ p'_k(t) - p'_{*k} \end{array} \right) = \left( \begin{array}{cc} \cos \mu_k t & \sin \mu_k t \\ -\sin \mu_k t & \cos \mu_k t \end{array} \right) \left( \begin{array}{c} q'_0 \xi_k - q'_{*0} \xi_k \\ p'_0 \xi_k - p'_{*0} \xi_k \end{array} \right). \tag{39}
\]

The solution of the original system is recovered performing the inverse transformation \( x = S_H x' \) for \( x'(t) \) in Eq. (35), which is precisely Eq. (28) since

\[
S_t = \exp[J H t] = \exp[J S_H^{-1} A_H S_H^{-T} t] \exp[S_H J A_H S_H^{-T} t] = S_H^T \exp[J A_H t] S_H^{-T} = S_H^T S'_t S_H^{-T}. \tag{40}
\]

As a last comment, the Hamiltonian in Eq. (26) can be conveniently rewritten as

\[
H(x) = \frac{1}{2} (x - x_*) \cdot H(x - x_*) - \frac{1}{2} \xi \cdot H^{-1} \xi + H_0. \tag{41}
\]

and the affine transformation

\[
x'' = S_H^T (x - x_*) \tag{42}
\]

reduces the above Hamiltonian to \( H''(x'') = \frac{1}{2} (x'') \cdot A_H x'' + H'_0 \), which describes oscillations as in Eq. (32), but around the origin of phase space. The reason to keep the equilibrium coordinate \( x'_* \) in Eq. (32) is related to the study of small oscillations, where the Hamiltonian often has multiple fixed points and it may be interesting to analyze the behavior of the system around each of them, as will become clear soon. Nevertheless, \( H''(x'') \) can always be obtained performing the (canonical) rigid translation \( (x' - x'_*) \mapsto x'' \) in Eq. (32).

### B. Complex Phase-Space

The resemblance of Eq. (36) to the Euler formula, \( e^{i \theta} = \cos \theta + i \sin \theta \), is noticeable. In the former, the matrix \( J \) is such that \( J^2 = -I_{2n} \) and performs the role of the imaginary unity. The mechanical Euler-like behavior can be further explored by diagonalizing the matrix \( J A_H \):

\[
W(JA_H)W = i \left( \begin{array}{cc} \Omega & 0_n \\ 0_n & -\Omega \end{array} \right), \tag{43}
\]

where \( \Omega := \text{Diag}(\mu_1, \ldots, \mu_n) \) and the unitary matrix

\[
W := \frac{1}{\sqrt{2}} \left( \begin{array}{cc} I_n & i I_n \\ i I_n & I_n \end{array} \right) \tag{44}
\]

is symmetric \( W^T = W \). Note that \( W^T W^* = W^{-1} \) and \( W^T JW = J \). Last property is the condition (13) for the complex matrix \( W \), however the symplectic group is only defined for real matrices.

Considering the vectors \( q' = (q'_1, \ldots, q'_n)^T \) and \( p' = (p'_1, \ldots, p'_n)^T \), the canonical complex change of coordinates

\[
z := W x' = \frac{1}{\sqrt{2}} \left( \begin{array}{c} q' + ip' \\ ip' - q' \end{array} \right) \tag{45}
\]

transforms the equations of motion Eq. (35) to

\[
z(t) = \tilde{S}_t (z_0 - z_*) + z_*, \quad \tilde{S}_t := W S'_t W = e^{i \Omega t} \oplus e^{-i \Omega t}, \tag{46}
\]

where we used Eq. (43). Each component \( (k = 1, \ldots, n) \) in the previous equation evolves as \( (z_k(t) - z_{*k}) = e^{i \mu_k t} (z_0 - z_{*k}) \), which is the complex version of Eq. (39).

Despite complex, since \( W \in \text{Mat}(2n, \mathbb{C}) \), transformation Eq. (45) preserves not only the Poisson bracket, as in Eq. (25), but also the Hamilton’s equations, \( \dot{z} = \frac{\partial H}{\partial z} \), where \( \tilde{H} = H' (W^* x') \) with \( H' \) given by Eq. (32). As we shall see, transformation Eq. (45) is the bridge towards the creation-annihilation operators in quantum mechanics and the coordinates \( z \) are their classical counterpart.
C. The Problem of Small Oscillations

Consider a generic time-independent Hamiltonian $\hat{H}$ described by a smooth function $H(x)$. A fixed point of the system, denoted $x_*$, is an initial condition that does not evolve: $x(t) = x_*, \forall t \in \mathbb{R}$, which can be determined by the solution of

$$\dot{x} = 0 \iff \left. \frac{\partial H}{\partial x} \right|_{x=x_*} = 0. \quad (47)$$

The behavior of the system around the fixed point can be determined by a Taylor expansion up to second order:

$$H(x) \approx H(x_*) + \xi_*(x-x_*) + \frac{1}{2}(x-x_*) \cdot \mathbf{H}_*(x-x_*), \quad (48)$$

where

$$\xi_* := \left. \frac{\partial H}{\partial x} \right|_{x=x_*} \in \mathbb{R}^n,$$

$$\mathbf{H}_* := \left. \frac{\partial^2 H}{\partial x \partial \dot{x}} \right|_{x=x_*} \in \mathcal{M}(2n, \mathbb{R}). \quad (49)$$

This approximation leads to a quadratic Hamiltonian like Eq. (26) and the solution around the fixed point is determined by Eq. (28). If $\mathbf{H}_* > 0$, the movement of the system is described by the analysis already performed with the Williamson theorem.

In principle, the problem of small oscillations is solved as described in Sec. III A. However, it is worth emphasizing that the efficiency of the approximation Eq. (48) is only guaranteed if the trajectories of the original system always remain close to $x_*$, which is equivalent to saying that the fixed point is a stable center. For a quadratic Hamiltonian of the form Eq. (26), a necessary and sufficient condition for this stability is $\mathbf{H} > 0$. However, considering generic Hamiltonians, there are situations where the stability will depend on higher-order terms, which includes the case in which $\mathbf{H}_* = 0$, and the present theory does not apply. The analysis for generic systems is a subject of the Lyapunov stability theory and is far from the objectives of this paper.

Other kinds of expansions can be performed on a generic Hamiltonian and the Williamson theorem can be also useful to describe the behavior of the system. For instance, if the Hamiltonian depends on a parameter $\epsilon$, an expansion like

$$H(x, \epsilon) = \sum_{k=0}^{\infty} \frac{\epsilon^k}{k!} \frac{\partial^k H}{\partial \epsilon^k} \bigg|_{\epsilon=0} \quad (50)$$

will be structurally different from Eq. (48), although it can also provide a quadratic Hamiltonian up to truncated. The above stability discussion can be translated to the present case if the fixed points of the truncated expansion remain close to the ones of the original Hamiltonian.

In the Supplementary Material, the Lagrangian way of dealing with oscillations is straightforwardly developed and compared with the Hamiltonian description. The advantages of the latter becomes clear since the Williamson theorem applies to the general case.
Eq. (53). Indeed, \([\hat{x}_k \xi_k, \hat{x}_j] = \xi_k (\hat{x}_k \hat{x}_j - \hat{x}_j \hat{x}_k) = i\hbar J_{kj} \xi_k\) and
\[
[\hat{x}_k \mathbf{H}_{kl} \hat{x}_l, \hat{x}_j] = \mathbf{H}_{kl}(\hat{x}_k \hat{x}_j \hat{x}_j - \hat{x}_j \hat{x}_k \hat{x}_l) \\
= \mathbf{H}_{kl}(\hat{x}_k \hat{x}_j \hat{x}_j + i\hbar J_{kj} \hat{x}_k - \hat{x}_j \hat{x}_k \hat{x}_l) \\
= \mathbf{H}_{kl}(i\hbar J_{kj} \hat{x}_l + i\hbar J_{lj} \hat{x}_k) \\
= -i\hbar (J_{jk} \mathbf{H}_{kl} \hat{x}_l + J_{lj} \mathbf{H}_{lk} \hat{x}_k),
\] (56)
where last equality is attained using that \(\mathbf{H}^\top = \mathbf{H}\) and \(J^\top = -J\).

The Heisenberg equation in Eq. (55) is exactly the Hamilton equation, Eq. (27), with the 
replacement \(x \mapsto \hat{x}\). Thus, from Eq. (28), its solution is
\[
\hat{x}(t) = S_t(\hat{x}_0 + \mathbf{H}^{-1} \xi) - \mathbf{H}^{-1} \xi.
\] (57)

The very same treatment is suitable also for the general quadratic case, where \(\mathbf{H}\) may not be positive-definite, see the Supplementary Material

Quantum Normal Modes

For a positive-definite matrix \(\mathbf{H}\), the Williamson theorem can be applied as in Eq. (30), and the solution in Eq. (57) can be brought to the normal-mode coordinates through the symplectic transformation \(\hat{x}' := S^{-1}_h \hat{x}\). Indeed,
\[
\hat{x}'(t) = S^{-1}_h S_x(S^\top_h \hat{x}_0 + \mathbf{H}^{-1} \xi) - S^{-1}_h \mathbf{H}^{-1} \xi \\
= S'_x(\hat{x}'_0 - \hat{x}'_a) + x'_s,
\] (58)
where Eq. (40) was employed, \(S'_x\) is written in Eq. (36), and \(x'_s\) is defined below Eq. (32).

Thanks to the commutation relation, Eq. (53), which is responsible for the coincidence of the Heisenberg equation, Eq. (55), with the Hamilton equation, Eq. (27), all the treatment performed in Sec. IIIA is precisely the same: all equations and results remain valid through the quantization \(x \mapsto \hat{x}\). Equations (57) and (58) are only two examples of this fact. For instance, the reader is invited to perform the transformation \(\hat{x}' := S^{-1}_h \hat{x}\) on the Heisenberg equation, Eq. (55), to obtain the quantum counterpart of Eq. (34). This is also true when considering the problem of small oscillations: the description in Sec. III C can be rigorously translated to the quantum case when replacing the Hamiltonian by its quantum version \(\hbar = H(\hat{x})\) for a smooth function \(H\).

Quantum oscillators are generally treated in the framework of creation and annihilation operators\(^9-11\). For a system of \(n\) degrees of freedom, it is convenient to define a collective notation for these operators through the vector
\[
\hat{z} := \sqrt{\hbar} \begin{pmatrix} \hat{a}_1 \\ \vdots \\ \hat{a}_n \\ i\hat{a}_1^\dagger \\ \vdots \\ i\hat{a}_n^\dagger \end{pmatrix},
\] (59)
where \(\hat{a}_j\) (resp. \(\hat{a}_j^\dagger\)) is the creation (resp. annihilation) operator of an oscillator with mass \(m_j\) and frequency \(\omega_j\), namely, \(\hat{a}_j := \sqrt{\frac{m_j}{2\hbar}} \hat{q}_j + i\sqrt{\frac{1}{2m_j\omega_j}} \hat{p}_j\). Observe that the adjoint operation \(\dagger\) acting on the vector \(\hat{z}\) is twofold: it means the ordinary vector transposition together with the Hermitian conjugation of each vector component. In this way, the “scalar” product between two of these vectors, say \(\hat{z}\) and \(\hat{w}\), is
\[
\hat{z}^\dagger \hat{w} := \sum_{j=1}^n \hat{z}_j^\dagger \hat{w}_k,
\] (60)
and note that, for the operator \(\hat{x}\) in Eq. (51), \(\hat{x}^\dagger = \hat{x}^\top\).

The relation between \(\hat{z}\) and \(\hat{x}\) is the complex linear transformation
\[
\hat{z} = \mathbf{W} \mathbf{Z} \hat{x},
\] (61)
where \(\mathbf{W}\) is the unitary matrix in Eq. (44) and \(\mathbf{Z}\) is the real symmetric symplectic matrix
\[
\mathbf{Z} := \text{Diag}(\sqrt{m_1\omega_1}, ..., \sqrt{m_n\omega_n}, \frac{1}{\sqrt{m_1\omega_1}}, ..., \frac{1}{\sqrt{m_n\omega_n}}).
\] (62)
Since \(\mathbf{WJW} = \mathbf{J}\), the same steps in Eq. (54) lead from Eq. (53) to
\[
[\hat{z}_j, \hat{z}_k] = i\hbar J_{jk} \ (j, k = 1, ..., 2n),
\] (63)
which is equivalent to \([\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk}\), and shows that the complex “coordinates” \(\hat{z}\) constitute a canonical system. Note that \(\hat{z}\) has a very particular structure in Eq. (59); the factor \(\sqrt{\hbar}\) and the imaginary \(i\)'s explicitly written in this equation are responsible for the canonical structure of the commutation relation Eq. (63).

Matrix \(\mathbf{Z}\) represents a simultaneous change of units for position and momentum. It is useful for the construction of creation-annihilation operators related to given oscillators, which are characterized by a given set of masses and frequencies. Symplectically equivalent creation-annihilation operators can be constructed using \(\hat{x}' = \mathbf{W}\hat{s}\) for any symplectic \(\mathbf{S}\). In particular for \(\mathbf{S} = S_h^{-1}\), the vector operator \(\hat{x}' = \mathbf{WS}_h^{-\top} \hat{x}\) is the quantization of Eq. (45). It is important to stress that transformations Eq. (61) and Eq. (45) can be applied to any physical system described by coordinates and momenta, not only the oscillatory ones.
The Hamiltonian \( \hat{h} = H(\tilde{x}) \) with \( H \) given by Eq. (26) through the transformation Eq. (61) becomes \( \hat{h} = H(Z^{-1}W^* \tilde{z}) \). Noting that \( \tilde{x} \cdot \eta = \tilde{x}^T \eta = \tilde{z}^T \eta \) for any real vector \( \eta \), the new Hamiltonian can be written as

\[
\tilde{h} = \frac{1}{2} \tilde{z}^T \tilde{H} \tilde{z} + \tilde{z}^T \zeta + H_0,
\]

(64)

where

\[
\tilde{H} := (WZ^{-1})^T H (WZ^{-1})^T = H^\dagger \in M(2n, \mathbb{C}),
\]

\[
\zeta := (WZ^{-1}) \zeta \in \mathbb{C}^{2n}.
\]

Transformation Eq. (61) preserves the Hermitian character of the Hamiltonian, since \( \tilde{H}^\dagger = \tilde{H} \) and \( (\tilde{z}^T \tilde{H} \tilde{z})^\dagger = \tilde{z}^T \tilde{H}^\dagger \tilde{z} \) for the above defined vector \( \zeta \).

As before, the canonical structure in Eq. (63) ensures that the treatment for quadratic Hamiltonians is readily translated to the new set of variables \( \tilde{z} \); however, now with complex matrices and vectors. For instance, the solution Eq. (57) under the change of variables Eq. (61) becomes

\[
\tilde{z}(t) = \tilde{S}_t (\tilde{z}_0 - z_*) + z_*,
\]

(66)

where \( z_* := -\tilde{H}^{-1} \zeta \) and \( \tilde{S}_t := (WZ) S_t (WZ)^{-1} = e^{t\tilde{H}_t} \), for \( S_t \) in Eq. (28). Note that \( \tilde{S}_t^\dagger J \tilde{S}_t = J \).

The Williamson theorem is applicable only to real matrices and, once a system is described by a Hamiltonian written as Eq. (64), some adaptations are needed. Of course, the inverse of transformation Eq. (61) can always be applied to Eq. (64) and the transformed Hamiltonian could be analyzed as before. Nonetheless, a straightforward approach is desirable since creation-annihilation operators are ubiquitous in physics.

The real and complex Hessians in Eq. (65) are related by a congruence, thus \( \tilde{H} > 0 \iff H > 0 \). For a positive-definite \( H \), Eq. (15) is equivalent to

\[
\tilde{S}_t H \tilde{S}_t^\dagger = \Lambda H \tilde{W}^* \tilde{W} = \Lambda_H.
\]

(67)

where \( \tilde{S}_t := W(\Sigma_H Z) \tilde{W}^* \). The last diagonalization relation induces the change of variables

\[
\tilde{z}' := \tilde{S}_t^{-1} \tilde{z}
\]

(68)

to be implemented in solution Eq. (66). Noting that \( \tilde{S}_t^\dagger JHS_t^{-1} = J\Lambda_H \), the mentioned equation reads

\[
(\tilde{z}'(t) - z_*') = W \exp[J\Lambda_H t] W^* (\tilde{z}_0' - z_*) = (e^{i\Omega t} + e^{-i\Omega t})(\tilde{z}_0' - z_*)
\]

(69)

where \( \Omega := \text{Diag}(\mu_1, ..., \mu_n) \), the numbers \( \mu_k \) are the symplectic eigenvalues of \( H \), and

\[
\tilde{z}' = -\tilde{S}_t^{-1} \tilde{H}^{-1} \zeta = -\tilde{W} \tilde{S}_t^\dagger \tilde{H}^{-1} \zeta = -\tilde{W} x_*',
\]

(70)

for \( x_*' \) defined below Eq. (32). At the end, the evolution of the quantum normal modes is the quantization of Eq. (46).

The solution written in Eq. (69) only depends on the symplectic spectrum, which is invariant under real symplectic transformations. In particular, \( \Lambda_{ZH} = \Lambda_H \), and there is no need to bother with \( Z \) in Eq. (61). Note also that the symplectic spectrum, see Eq. (17), can be obtained directly from the Euclidean spectrum of \( \tilde{H} \), since \( \det(\tilde{H} - \lambda \tilde{I}_n) = \det(H - \lambda I_{2n}) \), which follows from \( W \tilde{W} = J \) and \( \det \tilde{W} = 1 \).

V. STATISTICAL MECHANICS

The state of a physical system when it attains the equilibrium with a thermal reservoir at absolute temperature \( T \) is described by the canonical density operator\(^{12-14}\)

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

(71)

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 \( Z_\beta \) provides the normalization of the state in the sense that \( \text{Tr} \hat{\rho}_T = 1 \).

Consider a quadratic Hamiltonian \( \hat{h} = H(\tilde{x}) \) for the function \( H \) in Eq. (26). As learnt in previous sections, the condition \( H > 0 \) ensures that the dynamics of a system describes a collection of harmonic oscillators in appropriate coordinates. In statistical physics\(^{12-14}\) it is customary to deal with the equilibrium properties of these systems in the language of creation-annihilation operators. To this end, the transformation

\[
\tilde{z} = \tilde{W} \tilde{S}_t^\dagger (\tilde{x} + H^{-1} \zeta),
\]

(72)

which is the composition of the complexification in Eq. (61) with \( L = \tilde{I} \), and the affine symplectic coordinate change in Eq. (42), will be applied to the system Hamiltonian. Indeed,

\[
\tilde{H}(\tilde{z}) := H(\tilde{S}_t \tilde{W}^* \tilde{z} - H^{-1} \zeta)
\]

\[
= \frac{1}{2} \tilde{z}^T \tilde{W} \Lambda_H \tilde{W}^* \tilde{z} + H'_0
\]

\[
= \sum_{k=1}^n h_{\mu_k} (\hat{a}^*_k \hat{a}_k + \frac{1}{2}) + H'_0,
\]

(73)

where \( H'_0 = -\frac{1}{2} \zeta \cdot H^{-1} \zeta + H_0 \) is the same constant as in Eq. (32).

The partition function Eq. (71) thus becomes

\[
Z_\beta = \text{Tr} \exp [-\beta \hat{H}(\tilde{z})] = \text{Tr} \exp [-\beta \tilde{H}(\tilde{z})]
\]

\[
= e^{-\beta H'_0} \text{Tr} \exp \left[ -\beta \sum_{k=1}^n h_{\mu_k} (\hat{a}^*_k \hat{a}_k + \frac{1}{2}) \right]
\]

\[
e^{-\beta H'_0} \prod_{k=1}^n Z_k,
\]

(74)

where \( Z_k \) is the partition function of one oscillator\(^{12-14}\): \( Z_k = \text{Tr} \exp \left[ -\beta h_{\mu_k} (\hat{a}^*_k \hat{a}_k + \frac{1}{2}) \right] = \frac{1}{2} \csc(h_\mu) \).

(75)
Consequently,
\[
Z_{\beta} = \frac{e^{-\beta H_0}}{2^n} \prod_{k=1}^{n} \text{csch} \left( \frac{1}{2} \beta \hbar \mu_k \right). \tag{76}
\]

Finally, the thermal state Eq. (71), using Eqs. (73) and (76) becomes
\[
\hat{\rho}_T = \hat{\rho}_T^{(1)} \otimes \cdots \otimes \hat{\rho}_T^{(n)}, \quad \hat{\rho}_T^{(j)} := \frac{e^{-\beta \hbar \mu_j (\hat{a}_j^0 + \frac{1}{2})}}{2 \text{csch} \left( \frac{1}{2} \beta \hbar \mu_j \right)}. \tag{77}
\]

By virtue of the Williamson theorem, the partition function Eq. (76) is written only in terms of the symplectic spectrum of the Hessian of the Hamiltonian, becoming an invariant quantity under symplectic transformations due to the natural invariance of the symplectic spectrum. As is clear in this equation, this theorem also reduces the partition function of the original system to the one of a collection of independent harmonic oscillators. The transformation in Eq. (72) moves the system to the normal-mode coordinates, where the eigenfrequencies are the symplectic eigenvalues.

The internal energy (or simply energy) of a thermodynamical system in equilibrium is the mean value of the Hamiltonian: \( U := \langle \hat{h} \rangle = \text{Tr} \langle \hat{h} \hat{\rho}_T \rangle \). A system is said to be thermodynamically stable if addition (subtraction) of heat on the system never decreases (increases) its temperature. Physically speaking, it is a very reasonable and intuitive property, since its violation implies that the system will never attain an equilibrium state with any other system or with a thermal bath. Mathematically, the thermal stability of matter is represented by the positivity of the heat capacity, which is proportional to the ratio of the injected heat and the variation of the temperature. For a system in the state Eq. (71), it is given by
\[
C = \frac{\partial U}{\partial T} = k_B \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z_{\beta} = \sum_{k=1}^{n} \frac{k_B^2 \mu_k^2}{\hbar^2} \text{csch}^2 \left( \frac{\hbar \mu_k}{2k_B T} \right), \tag{78}
\]
where the last equality was obtained using the partition function in Eq. (76). Consequently, all the Hamiltonians with a positive-definite Hessian are thermodynamically stable. Thermodynamical instability does occur; examples of systems presenting this anomalous behavior are discussed in Ref. 32. For quadratic Hamiltonians, the simplest example would be a negative definite Hessian, where the convergence of the trace in Eq. (74) would not happen; other examples for the divergence of the partition function in the quadratic scenario are analyzed in Ref. 33.

The invariance of the partition function under symplectic transformations is directly extended for all the thermodynamical functions that are derived from it. For instance, the internal energy can be written as
\[
U := \frac{\partial}{\partial \beta} \ln Z_{\beta}, \quad \text{Helmholtz free energy of the system is} \quad F := -k_B T \ln Z_{\beta}, \quad \text{and the entropy} \quad S = k_B \beta (U - F). \quad \text{Of course, the above heat capacity is also invariant. These are highly nontrivial conclusions and were only possible due to the Williamson theorem: at a first glance, two symplectically congruent Hamiltonians may appear very distinct from each other, however the thermodynamical behavior of the system will be the same since it only depends on the symplectic spectrum.}
\]

When the zero-point energy of the higher frequency oscillator is small compared to the thermal energy, \( \hbar \beta \mu_n = \hbar \mu_n / (k_B T) \ll 1 \), the classical limit is attained by the expansion of Eq. (76) in powers of \( (\hbar \beta \mu_k) \) up to first order:
\[
Z_{\beta} \rightarrow Z_{\beta}^c = \frac{(k_B T)^n e^{-\beta H_0}}{h^n \prod_{k=1}^{n} \mu_k} = e^{-\beta H_0 + \frac{\beta}{2} \xi \langle H \rangle} \tag{79}
\]
This limit is the classical partition function
\[
Z_{\beta}^c := \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d^nx \ e^{-\beta H(x)} \tag{80}
\]
of the classical Hamiltonian in Eq. (26) with \( H > 0 \). The above Gaussian integral is promptly performed after the canonical transformation in Eq. (42). As in the quantum case, all thermodynamical functions will only depend on the symplectic spectrum and will be also symplectically invariant.

VI. UNCERTAINTY PRINCIPLE

In quantum mechanics, incompatible observables — the ones represented by noncommuting operators — can not be determined with unlimited precision. This is a consequence of uncertainty relations. In this section, after some words about uncertainty relations, the application of the Williamson theorem in this new scenario will be performed to reveal invariant structures common to all physical states.

If a physical system is described by the state \( | \psi \rangle \in \mathcal{H} \), the mean-value of an operator \( \hat{A} \) in such state is defined by \( \langle \hat{A} \rangle := \langle \psi | \hat{A} | \psi \rangle \). Defining also a displaced observable as \( \Delta \hat{A} := \hat{A} - \langle \hat{A} \rangle \), the variance of measurements of \( \hat{A} \) is expressed as
\[
\langle \Delta \hat{A}^2 \rangle = \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2 \geq 0. \tag{81}
\]
If another operator, say \( \hat{B} \), is considered, measurements in the same state are constrained by
\[
\langle \Delta \hat{A}^2 \rangle \langle \Delta \hat{B}^2 \rangle \geq \frac{1}{4} \langle [\Delta \hat{A}, \Delta \hat{B}] \rangle^2 = \frac{1}{4} \langle [\Delta \hat{A}, \Delta \hat{B}] \rangle^2, \tag{82}
\]
where \( \{ \hat{A}, \hat{B} \} := \hat{A} \hat{B} + \hat{B} \hat{A} \). Relation (82), first derived by E. Schrödinger, is a sufficient condition to the Robertson inequality
\[
\langle \Delta \hat{A}^2 \rangle \langle \Delta \hat{B}^2 \rangle \geq \frac{1}{4} \langle [\Delta \hat{A}, \Delta \hat{B}] \rangle^2, \tag{83}
\]
since \( |\langle \{ \hat{A}, \hat{B} \} \rangle | \geq 0 \). This inequality and the one in Eq. (82) are valid for any two operators. Specially when these operators are position and momentum, Eq. (83) receives the name of Heisenberg\(^{34,35} \). For a one-degree-of-freedom system, labeled by \( j \), the commutation relation is \( [\hat{q}_j, \hat{p}_j] = i\hbar \) and, from Eq. (83), the Heisenberg uncertainty principle is written as

\[
\Xi_j := \langle \Delta \hat{q}_j^2 \rangle \langle \Delta \hat{p}_j^2 \rangle - \frac{\hbar^2}{4} \geq 0. \tag{84}
\]

For \( n \) independent systems or a system of \( n \) non-interacting degrees of freedom, each pair coordinate-momentum will obey an inequality in Eq. (82), or its weaker form Eq. (83), that is \( \Xi_j \geq 0 \) for \( j = 1, \ldots, n \). However, if the systems or the degrees of freedom are interacting, certainly there will be other correlations (covariances) such as \( \Delta \hat{q}_j \Delta \hat{q}_k, \Delta \hat{q}_j \Delta \hat{p}_k, \Delta \hat{p}_j \Delta \hat{q}_k, \Delta \hat{p}_j \Delta \hat{p}_k \), which are not taken into account by Eq. (84). For these remaining pairs of observables, other uncertainty relations can be derived from Eq. (82), summing up \( n(2n+1) \) dependent inequalities\(^{36} \). Thinking in a practical situation, if one possesses a set of data corresponding to mean-values, variances, and covariances of a system, the number of inequalities grows quadratically with \( n \). The Williamson theorem shows again a way to treat the cases for a generic number of degrees of freedom.

To this end, an uncertainty relation taking into account all the covariances of the system and generalized for mixed states will be constructed. Afterwards, a symplectic diagonalization will be performed through the Williamson theorem to determine the invariant characteristics of this uncertainty relation. The results within the next subsections were originally reported in Refs.\(^{15} \) and \(^{37} \), while the derivation of the generalized uncertainty relation, despite being inspired by the same works, follows a proper pedagogical way.

A. Robertson-Schrödinger Uncertainty Relation

In general, the state of a quantum system is mixed and described by a density operator\(^{38-44} \) \( \hat{\rho} \in \mathcal{H} \otimes \mathcal{H}^\dagger \), where \( \mathcal{H} \) is the Hilbert space of the system. The mean value of observables are calculated through \( \langle \hat{A} \rangle := \text{Tr}(\hat{\rho} \hat{A}) \) and the pure state case is recovered when \( \hat{\rho} = |\psi\rangle \langle \psi| \).

Writing as before \( \Delta \hat{x}_j = \hat{x}_j - \langle \hat{x}_j \rangle \) and using the commutator and the anti-commutator definitions, the identity

\[
\frac{1}{2} \{ \Delta \hat{x}_j, \Delta \hat{x}_k \} + \frac{1}{2} [\Delta \hat{x}_j, \Delta \hat{x}_k] = \Delta \hat{x}_j \Delta \hat{x}_k \tag{85}
\]

is trivially constructed. Using the commutation relation Eq. (53) and taking its mean value, this identity is rewritten as

\[
\mathbf{V} + \frac{i\hbar}{2} \mathbf{J} = \langle \Delta \hat{x} \Delta \hat{x}^\dagger \rangle, \tag{86}
\]

where \( \mathbf{V} \) is the \textit{covariance matrix} of the system, defined through the matrix elements

\[
V_{jk} := \frac{1}{2} \{ \langle \Delta \hat{x}_j \rangle, \langle \Delta \hat{x}_k \rangle \}, \tag{87}
\]

and \( \langle \Delta \hat{x} \Delta \hat{x}^\dagger \rangle \in \mathbb{M}(2n, \mathbb{R}) \) is the matrix with elements\(^{38} \)

\[
\langle \Delta \hat{x}_j \Delta \hat{x}_k^\dagger \rangle_{jk} := \langle \Delta \hat{x}_j \Delta \hat{x}_k \rangle.
\]

The next step towards the derivation of the new uncertainty relation is to prove that

\[
\langle \Delta \hat{x} \Delta \hat{x}^\dagger \rangle \geq 0, \tag{88}
\]

which is performed in the Supplementary Material\(^{39} \). Finally, the matrix version of the uncertainty relation is composed joining Eqs. (86), (87) and (88):

\[
\mathbf{\Delta} := \mathbf{V} + \frac{i\hbar}{2} \mathbf{J} \geq 0, \tag{89}
\]

which means that \( \mathbf{\Delta} \) is a Hermitian positive-semidefinite matrix. The covariance matrix, due solely by the commutation relation in Eq. (53), is constrained to such uncertainty relation.

For a diagonal covariance matrix,

\[
\mathbf{V} = \text{Diag}(\langle \Delta q_1^2 \rangle, \ldots, \langle \Delta q_n^2 \rangle, \langle \Delta p_1^2 \rangle, \ldots, \langle \Delta p_n^2 \rangle), \tag{90}
\]

the uncertainty relation in Eq. (89) can be easily stated in terms of the Euclidean eigenvalues of the matrix \( \mathbf{\Delta} \). These eigenvalues are given by

\[
\delta_j^\pm = -\frac{1}{2} (\langle \Delta q_j^2 \rangle + \langle \Delta p_j^2 \rangle) \\
\pm \frac{1}{2} \sqrt{(\langle \Delta q_j^2 \rangle + \langle \Delta p_j^2 \rangle)^2 - 4 \Xi_j}, \tag{91}
\]

where \( \Xi_j \) is the quantity in Eq. (83) and \( j = 1, \ldots, n \). The matrix \( \mathbf{\Delta} \) will be positive semidefinite if and only if \( \delta_j^+ \geq 0, \delta_j^- \geq 0, \forall j \), which reduces exactly to \( n \) conditions \( \Xi_j \geq 0 \) in Eq. (84). This shows the equivalence of the uncertainty relation Eq. (89) with \( n \) uncertainty relations for noninteracting degrees of freedom of the form Eq. (84). Remember, however, that Eq. (89) is defined for any mixed state, while the uncertainty relation Eq. (84) is written only for pure states.

B. Williamson Theorem and Symplectic Invariance

The covariance matrix in Eq. (87) can be rewritten as

\[
\mathbf{V} = \frac{1}{2} \langle \Delta \hat{x} \Delta \hat{x}^\dagger + (\Delta \hat{x} \Delta \hat{x}^\dagger) \rangle, \tag{92}
\]

which is a sum of two positive semidefinite matrices from Eq. (88), thus \( \mathbf{V} \geq 0 \). Consequently, \( \mathbf{V} > 0 \) if and only if \( \det \mathbf{V} \neq 0 \). In this case, by the Williamson theorem, it is possible to write \( S \mathbf{V} S^\dagger = \mathbf{\Lambda} \) and attain, from the uncertainty relation Eq. (89), that

\[
\mathbf{\Delta}' := S \mathbf{\Delta} S^\dagger = \mathbf{\Lambda} + \frac{i\hbar}{2} \mathbf{J} \geq 0, \tag{93}
\]
since $S_VJS_V^T = J$. Due to the fact that $\Lambda_V$ is diagonal, using the formula for the determinant of block matrices in Sec.II, it is easy to find the $2n$ Euclidean eigenvalues of the matrix $\Delta'$:

$$\delta_{j}^\pm = \mu_j \pm \frac{1}{2} \hbar \quad (j = 1, ..., n),$$

where $\mu_j$ are the symplectic eigenvalues of $V$, see Eq. (15). The positive-semidefiniteness of $\Delta'$ in Eq. (93) is thus guaranteed if and only if $\delta_{j}^+ \geq 0$ and $\delta_{j}^- \geq 0$, which is equivalent to saying that $\mu_j \geq \hbar/2, \forall j$. Note that these last conditions subsume the fact $V > 0$; that is, the positive-definiteness of $V$ is automatically satisfied for a state such that $\Delta \geq 0$.

The uncertainty relation in Eq. (89) can now be rephrased: a quantum system has all symplectic eigenvalues (of the covariance matrix) greater or equal than $\hbar/2$.

The invariance of the commutation relation in Eq. (54) shows that there is not a preferable set of operators $\hat{x}$ to describe the system. Consequently, the uncertainty relation as expressed in terms of symplectic eigenvalues is a structural property of the system, since the symplectic spectrum is also invariant under symplectic transformations. Thinking in terms of a symplectic change of coordinates, the transformation $\hat{x}' = S \hat{x}$ for $S \in \text{Sp}(2n, \mathbb{R})$ turns the covariance matrix, defined in Eq. (87), into

$$V'_{jk} = \frac{1}{2} \sum_{l,m=1}^{2n} S_{jl}S_{km} \langle \{ \Delta \hat{x}_l', \Delta \hat{x}_m' \} \rangle = (SVS^T)_{jk}. \quad (95)$$

Note that $V$ and $V' = SVS^T$ share the same symplectic spectrum. Defining also $\Delta' := S \Delta S^T$ for $\Delta$ in Eq. (89), thus, $\Delta' \geq 0$ if and only if $\Delta \geq 0$, which shows that the true important quantity is not the covariance matrix itself, but its symplectic spectrum.

If in Eq. (95) $S = S_V$, where $S_V V S_V^T = \Lambda_V$, the transformation moves the set of system operators to a new set where the covariance matrix is $V' = \Lambda_V$. In this case, both the variances in position and in momentum for the same degree of freedom are equal to a symplectic eigenvalue of $V$, i.e., $\langle \Delta \hat{x}_j'^2 \rangle = \langle \Delta \hat{p}_j'^2 \rangle = \mu_j$.

At the end, a classical covariance matrix is defined as $\nu_c := \frac{1}{2} (\Delta x \Delta x^T + (\Delta x \Delta x^T)^\dagger) = (\Delta x \Delta x^T) \in M(2n, \mathbb{R})$, where the mean-values are taken with respect to a classical probability density function on phase space$^{12-14}$. Since $M(2n, \mathbb{R}) \ni \Delta x \Delta x^T \geq 0$, thus $\nu_c \geq 0$. Contrary to the quantum case, the commutator between classical variables is always null, thus $\nu_c$ is not subjected to any uncertainty relation. Consequently, it is possible that $\det \nu_c = 0$, which represents an absolute precision of the measurement of an observable (a linear combination of positions and momentum), i.e., the variance of such observable is null. If $\det \nu_c > 0$, the Williamson theorem can be applied and the symplectic eigenvalues can attain any positive value.

An example of the uncertainty relation for thermal states is found in the Supplementary Material$^{16}$. VII. FINAL REMARKS

The widely known Williamson theorem is actually a small piece (case $\gamma$ in p.162 of Williamson’s original work$^{40}$). According to Arnol’d$^{41}$, D.M. Galin has collected and reinterpreted the Williamsom results in a classical mechanics point of view, which are thus summarized in Appendix 6 of book 1, and deals with all the possible normal forms of generic quadratic Hamiltonians.

A normal form is understood as the simplest form to which a Hamiltonian is brought by symplectic congruences. Here, the Hamiltonian Eq. (32) is the normal form of Eq. (26). In principle, the examples considered in this paper can be extended for more generic cases using the list of Galin. However, what makes the Williamson theorem useful, practical, and celebrated is the particular normal form attained through Eq. (15), which only works for positive-definite matrices. Although all the other normal forms are no longer diagonal, the structure of this paper and the basic concepts using symplectic theory serve as a starting point to the treatment of generic cases. For instance, statistical properties of systems governed by a generic quadratic Hamiltonian are described in Ref. 33 and constitute the generalization of the results in Sec.V. Surprisingly enough, not all of these are thermodynamically stable systems; however, the thermodynamical properties are symplectically invariant, like the stable case analyzed here.

To the interested reader, a detailed and introductory review on the symplectic formalism and its relation with quantum mechanics is Ref. 6, while advanced mathematical background, rigorous results, and the state of the art are found in Ref. 5. An enjoyable discussion of nontrivial consequences of symplectic geometry in classical and quantum mechanics is Ref. 25.

The applicability of the Williamson theorem is spread over physics and goes far beyond the presented subjects. The transformation in Eq. (68) is a multimode Bogoliubov transformation$^{41}$, an ubiquitous method in solid state physics, field theory and quantum optics. As a current research area in quantum information, entanglement is a genuine quantum property of composite (in our notation $n \geq 2$) and interacting systems. A relation almost equal to Eq. (89) is used to verify its existence$^{42}$. Again the Williamson theorem plays a fundamental role and symplectic eigenvalues are used to quantify how much a system is entangled$^{43}$. The very same procedure presented in Sec.IV is applied to describe the propagation of information, heat, classical and quantum correlations (e.g. entanglement) through bosonic chains in Ref. 44.

The author ultimately hopes that students, teachers, and researchers should face the developed subject as a new card up their sleeves, expanded far beyond the set of examples presented here.
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[30] To avoid misunderstandings, the operator \( \hat{q}_{j} \) is the position operator related to the \( j^{\text{th}} \) degree of freedom and is a short notation to \( \hat{q}_{j} \otimes \hat{1}_{2} \otimes \cdots \otimes \hat{1}_{j-1} \otimes \hat{q}_{j+1} \otimes \hat{1}_{j+2} \otimes \cdots \otimes \hat{1}_{n} \), where \( \hat{1}_{j} \) is the identity operator on the Hilbert space associated to the \( j^{\text{th}} \) degree of freedom. The same consideration applies to momenta operators.
[31] For a real vector \( \eta := (\eta_{1}, ..., \eta_{2n}) \in \mathbb{R}^{2n} \), the sum \( \sum_{j=1}^{2n} \eta \cdot A_{jk} \hat{x}_{j} \) is a vector with components \( \hat{x}'_{j} = \sum_{j=1}^{2n} A_{jk} \hat{x}_{k} \) for \( j = 1, ..., 2n \).
[31] In the scope of this work, it is enough to consider a canonical symmetric quantization, which consists in replacing products \( \hat{x}_j \hat{x}_k \) by its symmetric version \( \frac{1}{2}(\hat{x}_j \hat{x}_k + \hat{x}_k \hat{x}_j) \). Note that, incidentally, \( H^\dagger = H \) implies a symmetric quantization for the classical Hamiltonian in Eq. (26). The quantization of a classical system is itself an open problem of quantum mechanics, see S.T. Ali and M. Engliš, “Quantization Methods: A Guide for Physicists and Analysts,” Rev. Math. Phys. 17(4), 391-490 (2005).

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Supplementary Material on
“Williamson theorem in classical, quantum, and statistical physics”

This Supplementary Material contains 1. A pedagogical proof for the Williamson Theorem (Sec.II of the main text); 2. An extension of the results in Sec.III of the main text for generic quadratic Hamiltonians; 3. The Lagrangian treatment of oscillations and comparison with the Hamiltonian case; 4. The demonstration of Eq.(88) in Sec.VI of the main text; 5. Three physical motivated examples for the application of the theorem.

Equations here are named as (SM-#), while references for equations in the main text appear as (#). This material contains its own bibliography at the end.

SM1. PROOF OF WILLIAMSON THEOREM

Mathematical definitions and properties of some objects in the Theorem and in the proof can be found in Sec.II of the main text. For convenience, the theorem is reproduced here.

Williamson theorem: Let \( M \in M(2n, \mathbb{R}) \) be symmetric and positive definite, i.e., \( M^\top = M > 0 \). There exists \( S_M \in Sp(2n, \mathbb{R}) \) such that

\[ S_M M S_M^\top = \Lambda_M, \]

\[ \Lambda_M := \text{Diag}(\mu_1, ..., \mu_n, \mu_1, ..., \mu_n) \]  

with \( 0 < \mu_j \leq \mu_k \) for \( j \leq k \). Each \( \mu_j \) is such that

\[ \det(JM \pm i\mu_j I_{2n}) = 0 \quad (j = 1, ..., n), \]

and the matrix \( S_M \) admits the decomposition

\[ S_M = \sqrt{\Lambda_M} O \sqrt{M}^{-1}, \]

where \( O \in M(2n, \mathbb{R}) \) satisfies

\[ O \sqrt{M} J \sqrt{M} O^\top = \Lambda_M J, \]

\[ O^\top = O^{-1}, \text{ i.e., is an orthogonal matrix.} \]

As a useful notation for the proof, the set containing all the Euclidean eigenvalues of a matrix \( A \), its spectrum, is denoted by \( \text{Spec}_\mathbb{C}(A) \). If all the Euclidean eigenvalues belong to the real set, \( \mathbb{K} = \mathbb{R} \), otherwise \( \mathbb{K} = \mathbb{C} \).

Proof: Consider a symmetric positive definite matrix \( M \in M(2n, \mathbb{R}) \). The matrix defined by \( \tilde{M} := \sqrt{M} J \sqrt{M} \in M(2n, \mathbb{R}) \), with

\[ J := \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix} \in M(2n, \mathbb{R}), \]

see Eq.(13), is anti-symmetric (\( \tilde{M}^\top = -\tilde{M} \)), since \( \sqrt{M} = \sqrt{\tilde{M}} \) and \( J^\top = -J \). It also has the same eigenvalues of \( JM \), since their characteristic polynomials are equal:

\[ P(\lambda) := \det(\tilde{M} - \lambda I_{2n}) = \sqrt{\det M} \det(J \sqrt{M} - \lambda \sqrt{M}^{-1}) = \det(JM - \lambda I_{2n}). \]

Thus, any property of the spectrum of the matrix \( \tilde{M} \) is shared by the spectrum of \( JM \).

Since \( \det \tilde{M} = \det(JM) = \det M \in \mathbb{R} \), complex eigenvalues of \( \tilde{M} \) come always in conjugate pairs, which is compactly expressed as

\[ \lambda \in \text{Spec}_\mathbb{C}(\tilde{M}) \iff \lambda^* \in \text{Spec}_\mathbb{C}(\tilde{M}). \]  

Using again the characteristic polynomial, but taking into account the anti-symmetry of \( \tilde{M} \), one has

\[ P(\lambda) = \det(\tilde{M} - \lambda I_{2n}) = \det(\tilde{M} - \lambda I_{2n})^\top = \det(\tilde{M}^\top - \lambda I_{2n}) = (-1)^{2n} \det(\tilde{M} + \lambda I_{2n}), \]

i.e., \( P(\lambda) = P(-\lambda) \), or the eigenvalues come also in symmetric pairs:

\[ \lambda \in \text{Spec}_\mathbb{C}(\tilde{M}) \iff -\lambda \in \text{Spec}_\mathbb{C}(\tilde{M}). \]

If \( \lambda \in \text{Spec}_\mathbb{C}(\tilde{M}) \), then \( \lambda^2 \) is an eigenvalue of the matrix \( \tilde{M}^2 \). However, \( \tilde{M}^2 = \sqrt{M} J M \sqrt{M} \) is a real symmetric matrix, thus possessing only real eigenvalues:

\[ \lambda \in \text{Spec}_\mathbb{C}(\tilde{M}) \implies \lambda^2 \in \text{Spec}_\mathbb{R}(\tilde{M}^2) \subseteq \mathbb{R}. \]

Taking together conditions (SM-7) and (SM-10), an eigenvalue of \( \tilde{M} \) must be a pure imaginary number:

\[ \lambda \in \text{Spec}_\mathbb{C}(\tilde{M}) \implies \lambda = i\mu, \quad \mu \in \mathbb{R}. \]

Taking into account condition (SM-9), the spectrum of \( M \) is

\[ \text{Spec}_\mathbb{C}(M) = \{i\mu_1, -i\mu_1, ..., i\mu_n, -i\mu_n\}, \]

where \( \mu_k \in \mathbb{R} \forall k \). The assertion in (SM-2) of the theorem is thus proved, since Eq.(SM-6) shows that \( \text{Spec}_\mathbb{C}(JM) = \text{Spec}_\mathbb{C}(M) \).

Returning to the matrix \( M^2 \), its symmetricity also ensures that there exist an orthogonal matrix \( O \in M(2n, \mathbb{R}) \), \( O^\top = O^{-1} \), such that

\[ O \tilde{M}^2 O^\top = D, \]  

(SM-13)
where $D$ is the diagonal matrix containing the real eigenvalues of $M^2$; from condition (SM-10), these eigenvalues are the square of the ones in (SM-12) and the columns of the matrix $O$ can be organized such that

$$D = -\text{Diag}(\mu_1^2, ..., \mu_n^2, \mu_1^2, ..., \mu_n^2).$$  \hspace{1cm} (SM-14)$$

Explicitly writing $M^2 = \sqrt{M}JMJ\sqrt{M}$, and rearranging terms in Eq.(SM-13), one can rewrite it as

$$S_M^{-T}JMJS_M^{-1} = -\Lambda_M.$$  \hspace{1cm} (SM-15)$$

for $S_M$ in (SM-3) and $\Lambda_M$ in (SM-1). Now, assuming that $S_M$ is a symplectic matrix, see Eq.(13), $S_M^{-T}J = JS_M$, Eq.(SM-15) becomes

$$S_MJS_M = -J^T\Lambda_MJ^T = \Lambda_M.$$  \hspace{1cm} (SM-16)$$

which proves Eq.(SM-1). However, it is still necessary to prove that $S_M$ is a symplectic matrix if and only if the matrix $O$ satisfies Eq.(SM-4), which goes as follows.

From the symplectic condition for $S_M$ written as Eq.(SM-3), and noting that $[\sqrt{\Lambda_M}, J] = [\Lambda_M, J] = 0$, one obtains

$$S_MJS_M = J \iff \sqrt{M}^{-1}O^T\sqrt{\Lambda_M}J\sqrt{\Lambda_M}O\sqrt{M}^{-1} = J \iff O^T\Lambda_MJ0 = \sqrt{M}J\sqrt{M} \iff \Lambda_M = O\sqrt{M}J\sqrt{M}O^T,$$

which is precisely Eq.(SM-4). Note that the matrix $O$ satisfying Eq.(SM-4) also satisfies Eq.(SM-13), since the last can be rewritten as

$$s^T(MO)^T(Os) = (J\Lambda_M)^2 = -\Lambda_k^2 = D_k.$$  \hspace{1cm} (SM-17)$$

consequently, this is the matrix composed by the orthonormal eigenvectors, respectively associated to the eigenvalues in (SM-14), of the symmetric matrix $M^2$.

Note also that the matrix $\Gamma := O\sqrt{M}^{-1}J\Lambda_M = O\sqrt{M}JM\sqrt{M}O - J\Lambda_M \in M(2n, \mathbb{R})$ is antisymmetric, $\Gamma^T = -\Gamma$, thus $\Gamma = 0_{2n}$ is a system of $n(2n-1)$ independent equations, which can be solved for the matrix elements of $O$. Since $O$ is orthogonal, it has $n(2n-1)$ independent matrix elements, and thus the system of equations can be solved for these unknowns. It only remains to prove that $\mu_k > 0, \forall k$. Since $M$ is positive-definite and is related to $\Lambda_M$ through a congruence, $S_MMS_M^{-1}$, thus, $\Lambda_M$ is also positive definite, and the theorem is proved.

**SM2. GENERIC QUADRATIC HAMILTONIANS**

The state of a mechanical system with $n$ degrees of freedom is described by a point in the $2n$-dimensional phase-space $\mathbb{R}^{2n} \times \mathbb{R}^n$ and the Hamiltonian of the system is, in principle, a generic smooth function

$$H : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R} : (q, p, t) \rightarrow h.$$  \hspace{1cm} (SM-18)$$

A mere rearrangement of the usual Hamilton equations,

$$\dot{q}_j = \partial h/\partial p_j, \quad \dot{p}_j = -\partial h/\partial q_j,$$  \hspace{1cm} (SM-19)$$

attains the compact form

$$\dot{x}_k = \sum_{l=1}^{n} J_{kl} \frac{\partial h}{\partial x_l},$$  \hspace{1cm} (SM-20)$$

for a column vector $x \in \mathbb{R}^{2n}$ and the matrix $J$ in (SM-5).

From the theory of ordinary differential equations (SM2), $\dot{x} = JHx + J\xi$ [Eq.(27)] is a first order nonhomogeneous linear equation with constant coefficients. Its solution is expressed by matrix exponentiation. The exponential of a matrix $A \in M(n, \mathbb{R})$ is defined by the Taylor series:

$$\sum_{k=0}^{\infty} A^k/k! =: \exp(A) \in M(n, \mathbb{R}).$$  \hspace{1cm} (SM-21)$$

For a generic matrix $H$, the solution of Eq.(27) is

$$x(t) = S_t x_0 + \int_{0}^{t} d\tau S_{\tau} J\xi,$$  \hspace{1cm} (SM-22)$$

with

$$S_t := \exp[JHt] \in Sp(2n, \mathbb{R}),$$  \hspace{1cm} (SM-23)$$

and can be checked by direct substitution.

For a nonsingular $H$, which is the case when $H > 0$, the above integral can be explicitly performed,

$$\int_{0}^{t} d\tau S_{\tau} = (S_t - I_2n)(JH)^{-1},$$  \hspace{1cm} (SM-24)$$

and solution (28) is attained.

**SM3. OSCILLATIONS IN LAGRANGIAN MECHANICS**

The treatment of oscillations traditionally departs from a Lagrangian function and consists of an expansion around a critical point of the potential energy of the system, leading to an approximated Lagrangian of the form

$$L(q, \dot{q}) = \frac{1}{2} \dot{q} \cdot T \dot{q} - \frac{1}{2} q \cdot Uq,$$  \hspace{1cm} (SM-25)$$

where $q = (q_1, ..., q_n)^T$ is the vector of the generalized coordinates, $\dot{q} = dq/dt$ are the generalized velocities, and $T, U$ are real symmetric matrices. The standard recipe follows a long procedure to simultaneously diagonalize the matrices $T$ and $U$, attaining a Lagrangian of oscillators if both $T > 0$ and $U > 0$. In order to compare with the Hamiltonian treatment presented so far, a straightforward Lagrangian approach will be developed.

If $T > 0$ and $U > 0$, it is possible to define the symmetric matrix $\tilde{U} := \sqrt{T^{-1}}U\sqrt{T^{-1}}$, which is a congruence of
the matrix \( U \), thus also positive-definite, \( \tilde{U} > 0 \). Consider now, the orthogonal matrix \( \hat{O} \) that diagonalizes \( \tilde{U} \),

\[
\hat{O} \tilde{U} \hat{O}^\top = \mathbf{Y} := \text{Diag}(u_1, \ldots, u_n), \tag{SM-26}
\]

where \( u_1 \leq u_2 \ldots \leq u_n \). The eigenvalues \( u_k \) are the roots of the characteristic polynomial

\[
det(\tilde{U} - \lambda I_n) = \det(U - \lambda T) \det(T^{-1}) = 0, \tag{SM-27}
\]

and are positive, \( u_k > 0, \forall k \), since \( \tilde{U} > 0 \).

According to the diagonalization of the matrix \( \tilde{U} \), the (point) transformation \( q' = \hat{O} \sqrt{T} q \) transforms Lagrangian (SM-25) into a new one describing \( n \) independent harmonic oscillators:

\[
L'(q', \dot{q}') = \frac{1}{2} \sqrt{T} \hat{O}^\top \mathbf{q}' \cdot T \sqrt{T} \hat{O} \mathbf{T} \hat{O}^\top \mathbf{T} \hat{O}^\top \mathbf{q}' + \frac{1}{2} \mathbf{q}' \cdot \mathbf{T} \hat{O}^\top \mathbf{T} \hat{O}^\top \mathbf{T} \hat{O}^\top \mathbf{q}'
\]

\[
= \frac{1}{2} q' \cdot \mathbf{q}' - \frac{1}{2} q' \cdot \mathbf{Y} q', \tag{SM-28}
\]

which is the desired result.

To show the equivalence with the Hamiltonian prescription, a Legendre transformation is performed in (SM-25):

\[
H(q, p) := p \cdot \dot{q} - L(q, \dot{q}) = \frac{1}{2} p \cdot T^{-1} p + \frac{1}{2} \mathbf{q} \cdot U \mathbf{q}, \tag{SM-29}
\]

where \( p := \partial L / \partial \dot{q} = T \dot{q} \). This Hamiltonian can be written as the quadratic form (26) with

\[
H = \begin{pmatrix} U & 0_n \\ 0_n & T^{-1} \end{pmatrix} > 0, \quad \mathbf{J} H = \begin{pmatrix} 0_n & T^{-1} \\ -U & 0_n \end{pmatrix}. \tag{SM-30}
\]

Noting that \( \det(\mathbf{J} H - \lambda I_{2n}) = \det(U + \lambda^2 T) \det(T^{-1}) \), Eq.(16) and Eq.(SM-27) show that \( u_k = \mu_k^2 \). Following (32), the normal-mode Hamiltonian is

\[
H'(x') = \frac{1}{2} p' \cdot \sqrt{\mathbf{Y}} p' + \frac{1}{2} q' \cdot \sqrt{\mathbf{Y}} q', \tag{SM-31}
\]

which actually is not the Legendre transformation of Lagrangian (SM-28). However, the symplectic transformation \( x'' = (\mathbf{Y}^{1/4} \oplus \mathbf{Y}^{-1/4}) x' \) gives rise to \( H''(x'') = \frac{1}{2} p'' \cdot p'' + \frac{1}{2} q'' \cdot \mathbf{Y} q'' \). Finally, the Hamiltonian \( H''(x'') \) is the Legendre transformation of Lagrangian (SM-28) and, consequently, the Williamson theorem (supplied by an extra symplectic transformation) provides the results of the standard methods.

The main advantage of the Hamiltonian description is the symplectic structure of phase space, where coordinates and momenta are treated on an equal footing. While the Lagrangian description departs from a separable form \( L = T - U \), the Hamiltonian is a generic function of phase-space coordinates, not restricted to \( T + U \). This is clearly manifested by the Hamiltonian (SM-29), which is a particular instance of the general quadratic case in Eq.(26).

**SM4. DEMONSTRATION OF EQ.(88)**

The spectral decomposition of the density operator \( \hat{\rho} \) reads

\[
\hat{\rho} = \sum_i p_i |\phi_i\rangle \langle \phi_i|, \quad \sum_i p_i = 1, \quad 0 \leq p_i \leq 1, \forall i, \tag{SM-32}
\]

where \( |\phi_i\rangle \in \mathcal{H} \) are the eigenvectors of \( \hat{\rho} \) associated to the eigenvalues \( p_i \). Employing such a decomposition, one obtains

\[
\langle \Delta \hat{x}_j \Delta \hat{x}_k \rangle = \text{Tr}(\hat{\rho} \Delta \hat{x}_j \Delta \hat{x}_k) = \sum_i p_i \langle \phi_i | \Delta \hat{x}_j \Delta \hat{x}_k | \phi_i \rangle; \tag{SM-33}
\]

using a completeness relation for a generic complete basis \( |\psi_m\rangle \in \mathcal{H} \), last equation becomes

\[
\langle \Delta \hat{x}_j \Delta \hat{x}_k \rangle = \sum_{l,m} p_l \langle \phi_l | \Delta \hat{x}_j | \psi_m \rangle \langle \psi_m | \Delta \hat{x}_k | \phi_l \rangle = \sum_{l,m} p_l \sum_{j,k} w_{(lm)j}^l w_{(lm)k}^l \tag{SM-34}
\]

where \( w_{(lm)j} := \langle \phi_l | \Delta \hat{x}_j | \psi_m \rangle \in \mathbb{C} \) is the component \( j \) of the vector \( w_{(lm)} := \langle \phi_l | \Delta \hat{x}_j | \psi_m \rangle \in \mathbb{C}^{2n} \). For any \( (l, m) \), the matrix \( w_{(lm)} w_{(lm)}^\dagger \geq 0 \), consequently it is possible to conclude that

\[
\langle \Delta \hat{x} \Delta \hat{x}^\top \rangle = \sum_{l,m} p_l w_{(lm)} w_{(lm)}^\dagger \geq 0, \tag{SM-35}
\]

since \( p_l \geq 0, \forall l \), as it was to be proved.

**SM5. EXAMPLES**

Three examples will be presented in this section. The objective of the first one is to compare the results provided by the Williamson theorem and the diagonalization of the Lagrangian function. It is designedly written to be independent of the main body of the text, in such a way that the reader would be able to understand the comparison without technical details.

The second example considers the process of symplectic diagonalization of a nontrivial Hamiltonian, which the main objective is to show how to perform in practice its symplectic diagonalization. Once the symplectic spectrum and the symplectic diagonalizing matrix are obtained, the determination of the normal modes of the system, both classical and quantum, are immediate, as well as the thermal equilibrium state.

In the third example, the uncertainty relations for thermal states associated to quadratic Hamiltonians will be examined, as well as the relation between the symplectic spectrum of the Hamiltonian and the one for the covariance matrix of the state.

**A. Interacting Trapped Ions**

The actual technological scenario is marked by an unprecedented control of quantum systems. Among
them, a single ion is confined inside a trap designed by (time-dependent) electromagnetic fields, a setup called Paul Trap\textsuperscript{SM3} in honor of its inventor and Nobel prize awarded. This setup combined with laser tech\textsuperscript{SM4} is the most developed setup for investigation of quantum effects and an imminent candidate for the construction of a quantum computer\textsuperscript{SM5}. In a linear trap\textsuperscript{SM3}, the center of mass of the ion is confined to move harmonically in one dimension and, since ions are charged (usually cations), two of them will interact electrically, see Fig.SM1.

![Diagram showing two trapped ions](Image)

Figure SM1. (color online) Pictorial representation of two interacting trapped ions. A parabola represents the confinement of one ion to the one-dimensional harmonic motion, while the wavelike curve represents the electrical interaction between the pair. The coordinates of the center of mass of each ion are denoted by $q_j$, while $q_{0j}$ and $\delta q_j := q_j - q_{0j}$ are, respectively, the equilibrium position (of each trap) and the displacement of the equilibrium when no electrical interaction (due to the other ion) is present. The distance between the traps are $d = q_{02} - q_{01}$. This system is inspired by the work in Ref.SM6.

A classical description for the system consists of two particles ($j = 1, 2$) with mass $m$, subjected to a harmonic potential with frequency $\omega$ (the frequency is determined by the trap), such that the kinetic energy is

$$T = \frac{m}{2} (\dot{q}_1^2 + \dot{q}_2^2).$$

The potential energy of the system, taking into account the trapping and the electrical interaction, is

$$U = \frac{m \omega^2}{2} (\delta q_1^2 + \delta q_2^2) + \frac{C}{|q_1 - q_2|},$$

where $C := K_e Q_1 Q_2$ for the electrostatic constant $K_e$, and the ionic charges $Q_1, Q_2$.

If the distance between the traps is much bigger than the displacements of the ions inside the traps, $d \gg \delta q_j$, an expansion of the electrostatic potential\textsuperscript{SM6} can be performed using $q_1 - q_0 = \delta q_1 - \delta q_2 - d$, that is

$$|\delta q_1 - \delta q_2 - d|^{-1} = \sum_{k=0}^{\infty} \frac{(\delta q_1 - \delta q_2)^k}{d^{k+1}}.$$  

Keeping only terms up to second order in this expansion, the potential energy becomes

$$U \approx \frac{1}{2} (q - q_*) \cdot U(q - q_*) + U_0,$$  

where $q := (q_1, q_2)^T$ is the column vector of the coordinates and the potential matrix is

$$U := \left( \begin{array}{cc} m \omega^2 + 2 \frac{C}{d} & -2 \frac{C}{d} \\ -2 \frac{C}{d} & m \omega^2 + 2 \frac{C}{d} \end{array} \right).$$

The equilibrium coordinate, $q_*$, for the potential energy (SM-39) is the solution of

$$U(q_* - q_0) = -\frac{C}{d} \left( \begin{array}{c} 1 \\ -1 \end{array} \right),$$  

for $q_0 := (q_{01}, q_{02})^T$. The potential offset is

$$U_0 := C/d - \frac{1}{2} (q_* - q_0) \cdot U(q_* - q_0).$$

One can then perform the point transformation

$$q' = \sqrt{m} \tilde{O}(q - q_*),$$

where $\tilde{O}$ is the orthogonal matrix, $\tilde{O}^T = \tilde{O}^{-1}$, that diagonalizes $U$. Such transformation always exists, since the potential matrix in (SM-40) is real and symmetric\textsuperscript{SM6}. Indeed,

$$\tilde{O} U \tilde{O}^T = \text{Diag} \left( m \omega^2, m \omega^2 + 4 \frac{C}{d^3} \right).$$

The new Lagrangian becomes

$$L'(q', \dot{q}') = \frac{1}{2} \dot{q}'^T \dot{q}' - \frac{1}{2} q' \cdot \Omega^2 q' + U_0$$

$$= \frac{1}{2} \sum_{k=1,2} (q_k'^2 - \omega_k^2 q_k^2) + U_0,$$

where $\Omega := \text{Diag}(\omega_1, \omega_2)$ and

$$\omega_1 := \frac{\omega}{m \omega^2 + 4 \frac{C}{d^3}}, \quad \omega_2 := \frac{1}{\omega_1},$$

Finally, from the Euler-Lagrange equation, one obtains

$$\ddot{q}_k + \omega_k^2 q_k = 0 \quad (k = 1, 2).$$

Despite the usual traps deal with cations, theoretically it is possible to consider generic charges in (SM-37). When the charges of the ions have the same sign ($C > 0$), then $\omega_k > 0$, and the movement will be oscillatory. In this case, $\det U > 0$ and the fixed point in (SM-43) is expressed as

$$q_* = q_0 - \frac{C}{d} U^{-1} (\begin{array}{c} 1 \\ -1 \end{array}) = q_0 - \frac{C m \omega^2}{d \det U} (\begin{array}{c} 1 \\ -1 \end{array}),$$

where $\tilde{O}$ is the solution of (SM-39).
which means that ion 1 (resp. 2) oscillates around a stable equilibrium point translated to the left (resp. right) with respect to the center of its trap $q_{01}$ (resp. $q_{02}$), according to the mutual repulsion of the charges.

In the other case, $C < 0$, the ions will attract each other and the movement will be stable (oscillatory evolution) only if $\omega^2 > 0$, that is, if $x^2 > 4|C|/(md^4)$. The stable fixed $q$, point will be displaced in the opposite direction of the previous case, due to the attraction. On the other hand, if $x^2 < 4|C|/(md^4)$, the equilibrium will be unstable since $\omega^2 < 0$, and the movement will be stable (oscillatory evolution) due to the attraction. On the other hand, if $x^2 < 4|C|/(md^4)$, the equilibrium will be unstable since $\omega^2 < 0$, thus solution $q_2(t)$ in (SM-48) is such that $\lim_{t \to \infty} q_2(t) = \infty$, which means that the trap collapses.

From the point of view of the Hamiltonian dynamics, the Hamiltonian of the original system is:

$$H(q, p) = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{m\omega^2}{2}(\delta q_1^2 + \delta q_2^2) + C |q_1 - q_2|,$$

and the same expansion in (SM-38) is performed to attain the Legendre transform of (SM-43), which can be written as:

$$H(x) = \frac{1}{2}(x - x_*) \cdot H(x - x_*) + U_0,$$  

with $x := (q_1, q_2, p_1, p_2)^\top$, similarly for $x_*$, and $H = m^{-1}I_2 \otimes U_0$.

In the Lagrangian scenario, the movement will be stable if the eigenvalues of $U_0$ are positive, which is the same to say that $U_0$ is (symmetric) positive-definite, observe that the positivity character of $U_0$ implies that $H$ above is also positive-definite. Departing from this fact, the matrix $S_H := L(\hat{O}^T \oplus \hat{O})$ is such that:

$$S_H H S_H^T = L(\hat{O}^T \oplus \hat{O}) H(\hat{O}^T \oplus \hat{O}) L^T = L \left[ (m^{-1}I_2) \oplus \text{Diag}(m\omega_1^2, m\omega_2^2) \right] L$$

$$= \text{Diag}(\omega_1, \omega_2, \omega_1, \omega_2),$$

where

$$L := \text{Diag} \left( \sqrt{m\omega_1}, \sqrt{m\omega_2}, \frac{1}{\sqrt{m\omega_1}}, \frac{1}{\sqrt{m\omega_2}} \right).$$

Despite being a toy model, in principle it can be reproduced in a quantum optics lab. The Hamiltonian $H_0$ governs the evolution of three noninteracting electromagnetic fields ("harmonic oscillators") with equal frequency $\omega$; all the other terms are related to the phenomenon known as squeezing, which can be reproduced experimentally by (nonlinear) interactions of the electromagnetic field with crystals. The Hamiltonian $H_1$ represents the squeezing on each electromagnetic field and is known as "one-mode squeezing", while the terms in $H_2$ are called "two-mode squeezing", since each term acts on pairs, and is responsible for the creation of entanglement between these field pairs.

Using transformation (59) with $m_j = 1, \omega_j = 1, \forall j$ (in suitable units of the problem), the Hamiltonian is rewritten as $\hat{H} = \hat{H}(\hat{x})$ for the function $H$ in (26) with $\xi = 0, H_0 = 0$ and

$$H = \begin{pmatrix} \omega \mathbf{I}_3 & C \mathbf{C} \\ C \mathbf{C} & \omega \mathbf{I}_3 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & -\kappa & \kappa \\ \kappa & 0 & -\kappa \\ \kappa & -\kappa & 0 \end{pmatrix}. $$

To obtain the normal modes of the system in question, it is necessary first to check whether the (symmetric) matrix $H$ is positive-definite. To this end, the Euclidean eigenvalues of $H$ are determined by roots of the characteristic polynomial $\det(H - \lambda I_2) = 0$, which are organized on the following diagonal matrix

$$D = \text{Diag}(\omega + \gamma, \omega - \kappa + \gamma, \omega + \kappa + \gamma, \omega - \gamma, \omega + \kappa - \gamma, \omega - \gamma - \kappa).$$

Since a symmetric matrix is positive definite if and only if its eigenvalues are positive, $\omega > \kappa + \gamma$ is a necessary
and sufficient condition for the positive definiteness of $H$. Considering that this is the case, the determination of the normal modes of this system is routed by the Williamson theorem.

The first step now is to determine the symplectic spectrum of $H$ following (SM-2); thus, solving for the roots of the characteristic polynomial $\det(HJ - \mu I_{2n}) = 0$, one finds $\Lambda_H = \text{Diag}(\mu_1, \mu_2, \mu_3, \mu_1, \mu_2, \mu_3)$, where

$$
\begin{align*}
\mu_1 &= \sqrt{\omega^2 - \gamma^2}, \\
\mu_2 &= \sqrt{\omega^2 - (\kappa - \gamma)^2}, \\
\mu_3 &= \sqrt{\omega^2 - (\kappa + \gamma)^2},
\end{align*}
$$

which are the eigenfrequencies of the system, or the frequency of the normal modes.

The next step is the determination of the symplectic matrix that symplectically diagonalizes $H$ as in (SM-3), but for that the square-root of $H^{-1}$ is needed. To calculate this square-root, the Euclidean diagonalization of $H$ will be performed.

Consider thus the orthogonal matrix $O'$ composed by the orthonormal eigenvectors of $H$, which are such that

$$
O'HO'^T = D,
$$

where $D$ is defined in (SM-57). The matrix $O'$ can be determined by brute force with the help of a symbolic computational program, if necessary, however, it is useful to show that it can be decomposed as the product of two suitable matrices:

$$
O' = R (O_C \oplus O_C),
$$

where

$$
R := \frac{1}{\sqrt{2}} \begin{pmatrix} I_3 & I_3 \\ -I_3 & I_3 \end{pmatrix}, \quad O_C := \begin{pmatrix} 1/2 & -i/\sqrt{2} & i/2 \\ i/2 & 0 & 1/2 \\ -i/2 & 1/\sqrt{2} & i/2 \end{pmatrix}.
$$

The orthogonal matrix $O_C$ is the one that performs the diagonalization of the symmetric matrix $C$ in Eq.(SM-56), i.e.,

$$
O_C CO_C^T = D_C := \text{Diag}(\gamma, \gamma - \kappa, \gamma + \kappa).
$$

With this in hand, the diagonalization of $H$ is performed in two steps, first by the diagonalization of the blocks $C$, and then by applying a rotation $R$:

$$
O'HO'^T = R \begin{pmatrix} \omega I_3 & O_C CO_C^T \\ O_C CO_C^T & \omega I_3 \end{pmatrix} R^T = \begin{pmatrix} \omega I_3 + D_C & 0 \\ 0 & \omega I_3 - D_C \end{pmatrix} = D.
$$

Note that $R^T = R^{-1}$, and $R \in \text{Sp}(6, \mathbb{R})$, also note that $(O_C \oplus O_C) \in \text{Sp}(6, \mathbb{R})$ and, consequently, $O'$ besides orthogonal is also symplectic.

The two step procedure in last paragraph only works due to $C^T = C$. As a clue, in practical problems, for instance, the ones in Ref.SM11, is common to find a Hamiltonian where the blocks can be diagonalized one at a time, and thus a final rotation can be used to diagonalize the whole matrix. This is the reason to illustrate it here. In the absence of this structure, or other symmetry like it, symbolic computational programs solves the problem with efficiency.

The symplectic matrix, which moves the system to normal-modes coordinates, from Eq.(SM-3), is given by $S_H = \sqrt{\Lambda_H} O \sqrt{H}^{-1}$. From (SM-59), one writes

$$
\sqrt{H^{-1}} = O' \sqrt{D^{-1}} O'^T,
$$

and it remains to determine the matrix $O$ from the solution of Eq.(SM-4), which for the present case is

$$
O \sqrt{H} J \sqrt{H} O^T = \Lambda_H J.
$$

Using again (SM-59) and the fact that $O' \in \text{Sp}(2n, \mathbb{R})$, then above equation becomes

$$
O' \sqrt{D} J \sqrt{D} O'^T O'^T = O' \Lambda_H J O'^T O'^T = \Lambda_H J
$$

thus $O = O'^T$ and the matrix $S_H$ becomes

$$
S_H = \sqrt{\Lambda_H} \sqrt{D^{-1}} O'^T,
$$

for $\Lambda_H$ in (SM-58), $D$ in (SM-57) and $O'$ in (SM-60).

With above matrix, the evolution of the normal mode coordinates is (35) for $x_\nu' = 0$ and $S_\nu'$ in (36) with $A_H$ in (SM-58). The thermal equilibrium state (71) for the system described by the Hamiltonian in (SM-55) can be written in terms of creation-annihilation operators using the symplectic change of variables in (72), with $S_H$ in (SM-65), $\xi = 0$, and $W$ in (44) for $n = 3$. The resulting expression is Eq.(77) for $n = 3$.

### C. Thermal State and Uncertainty Principle

As learnt in Sec.VIB, the uncertainty relation when written in terms of symplectic eigenvalues (of the covariance matrix) is a structural property of the system and is independent of an operator-basis choice. For a Thermal state described by (77), it is convenient to write the uncertainty relation (89) in terms of the creation-annihilation operators defined in (59).

To this end, it is opportune to deal with the eigenvectors of the Hamiltonian $\hbar \mu_j (\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2})$, which are Fock states denoted by $|\nu_j \rangle$ for $\nu_j = 0, ..., \infty; \nu_j$ an eigenstate of the whole system is the tensor product state $|\nu_1, ..., \nu_n \rangle := |\nu_1 \rangle \otimes \cdots \otimes |\nu_n \rangle$. Consequently, the mean value of a generic operator $\hat{A}$ is calculated through

$$
\langle \hat{A} \rangle = \text{Tr}(\hat{\rho}_T \hat{A}) = \sum_{\nu_1=1}^{\infty} \cdots \sum_{\nu_n=1}^{\infty} \langle \nu_1, ..., \nu_n | \hat{\rho}_T \hat{A} | \nu_1, ..., \nu_n \rangle.
$$
Defining $\Delta \hat{z} := \hat{z} - \langle \hat{z} \rangle$, see Sec. VI of the main text, the covariance matrix

$$\hat{V}_{jk} = \frac{1}{2} \text{Tr} \left[ (\Delta \hat{z}_j, \Delta \hat{z}_k) \hat{\rho}_T \right]$$

(SM-66)

for the thermal state in (77) is determined by calculating the following quantities:

$$\langle \hat{a}_j \rangle = \langle \hat{a}_j^\dagger \rangle = 0, \quad \langle \hat{a}_j \hat{a}_k \rangle = \langle \hat{a}_j^\dagger \hat{a}_k^\dagger \rangle = 0,$$

(SM-67)

and

$$\langle \hat{a}_j^\dagger \hat{a}_j \rangle = \sum_{\nu_j=0}^{\infty} \langle \nu_j | \hat{\rho}_T | \nu_j \rangle = \sum_{\nu_j=0}^{\infty} \nu_j e^{-\beta \hbar \nu_j} \left( e^{\frac{\beta \hbar \nu_j}{2}} - 1 \right)^{-1}.$$

Collecting all these mean-values into $\hat{V}$, see Eq.(59), one finds

$$\hat{V} = \frac{i\hbar}{2} \left( \begin{array}{cc} 0_n & \hat{N} \\ \hat{N} & 0_n \end{array} \right),$$

(SM-68)

where $\hat{N} := 2 \text{Diag}(\nu_1, ..., \nu_n) + I_n$ and

$$\nu_j : = \langle \hat{a}_j^\dagger \hat{a}_j \rangle = \left( e^{\beta \hbar \nu_j} - 1 \right)^{-1} \geq 0 \quad \text{(SM-69)}$$

is called the bosonic occupation number$^\text{SM13}$. Once the covariance matrix is obtained for the operators $\hat{z}$, it remains to write it for $\hat{x}$ through the transformation (72). First note that, from Eq.(SM-67), $\langle \hat{z} \rangle = 0$ and thus $\langle \hat{x} \rangle = -\mathbf{H}^{-1} \hat{z}$; consequently $\Delta \hat{z} = \mathbf{W} \hat{S}_H^T \Delta \hat{x}$. Inserting this last relation into the definition (SM-66), similarly to (95), one attains

$$\hat{V} = \mathbf{W} \hat{S}_H^T \hat{V} \hat{S}_H^{-1} \mathbf{W}.$$

(SM-70)

It is essential to note that, while $\hat{V}$ in (SM-70) is calculated with the thermal state written as in (77), matrix $\mathbf{V}$ should be calculated with the thermal state written for the quadratic Hamiltonian $\hat{h} = \mathbf{H}(\hat{z})$. This is a mere consequence of the fact that the Hamiltonian is subjected to the same transformation, see Eq.(73), as it should be.

Departing from the uncertainty relation (89), using Eq. (SM-70), and the fact that $\hat{S}_H$ is symplectic, the uncertainty relation becomes$^\text{SM14}$

$$\hat{S}_H^T \mathbf{W} \hat{V} \mathbf{W}^* \hat{S}_H + \frac{i\hbar}{2} \mathbf{J} \geq 0 \Longleftrightarrow \mathbf{W}^* \hat{V} \mathbf{W}^* + \frac{i\hbar}{2} \mathbf{J} \geq 0$$

$$\Longleftrightarrow \left( \begin{array}{cc} \hat{N} & I_n \\ -I_n & \hat{N} \end{array} \right) \geq 0,$$

where Eq.(SM-68) was employed. The Euclidean eigenvalues of the last matrix are given by $\lambda_j^\pm = 2\nu_j + 1 \pm 1$, $j = 1, ..., n$, which are all non-negative, since $\nu_j \geq 0$, see Eq.(SM-69). In conclusion, every positive-definite quadratic Hamiltonian generates a genuine physical thermal state.

By the end, note that since $\hat{V}$ is complex, it is not suitable for the Williamson theorem. However, it is still possible to determine the symplectic eigenvalues for the appropriate covariance matrix, which is $\mathbf{V}$. Writing explicitly $\mathbf{W}$, see Eq.(44), in Eq.(SM-70), one reaches

$$\mathbf{V} = \frac{i\hbar}{2} \hat{S}_H^T (\hat{N} \oplus \hat{N}) \hat{S}_H.$$  

(SM-71)

However, the symplectic spectrum is invariant under a symplectic congruence, in such a way $\Lambda_\mathbf{V} = \frac{i\hbar}{2} (\hat{N} \oplus \hat{N})$, thus the symplectic eigenvalues of the covariance matrix $\mathbf{V}$ are $\mu_j = \frac{i\hbar}{2} (2\nu_j + 1)$, $j = 1, ..., n$. Due to the definition of $\nu_j$ in Eq.(SM-69), the relation between the symplectic spectra of the Hamiltonian and the covariance matrix is

$$\Lambda_\mathbf{V} = \frac{i\hbar}{2} \text{coth} \left( \frac{1}{2} \beta \hbar \Lambda_H \right),$$

(SM-72)

which is valid for any positive-definite quadratic Hamiltonian.

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[SM7] If $\det \mathbf{U} \neq 0$, the solution for $q_\star$ is unique and given by $q_\star = q_0 - \frac{1}{2} \mathbf{U} \left( \begin{array}{c} 1 \\ -1 \end{array} \right)$; otherwise, there can be multiple equilibrium points $q_\star$.

[SM8] Implementing the point transformation $q_\prime = q - q_\star$, in (SM-43), this Lagrangian attains (SM-25) with $\mathbf{T} = m I_2$. The potential matrix in (SM-26) is thus $\mathbf{U} = m^{-1} \mathbf{U}$ and $\mathbf{O}$ is the diagonalizing matrix of $\mathbf{U}$.
Squeezing is a property related to the variances of measurements, see Eq. (81). Suppose that there is a quantum state such that \( \langle \Delta q_j^2 \rangle \langle \Delta p_j^2 \rangle = c \), where of course \( c \geq h^2/4 \), see Eq. (84). A new state is said squeezed with respect to the former if one of the variances is increased while the other is decreased by the same factor, that is, the new variances are such that \( \langle \Delta q'_j^2 \rangle = s^2 \langle \Delta q_j^2 \rangle \) and \( \langle \Delta p'_j^2 \rangle = s^{-2} \langle \Delta p_j^2 \rangle \). In a squeezed state, measurements of one variable will have a sharper distribution, while the one for the conjugate variable will be broader, however their product is left unchanged, \( \langle \Delta q'_j^2 \rangle \langle \Delta p'_j^2 \rangle = c \). For the quantum electromagnetic field, position and momentum are called quadrature and are identified by relations (59) and (61). The mentioned squeezing effect is generated by a Hamiltonian like \( \hat{H}_1 \) in Eq. (SM-55), while \( \hat{H}_2 \) generates the same effect but taking into account different fields.

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The transformation (SM-70) is not a congruence between \( \mathbf{V} \) and \( \tilde{\mathbf{V}} \) due to the matrices \( \mathbf{W} \). By the same reason, it is not possible to ensure that \( \mathbf{W} \Delta \mathbf{W} \) is a positive-definite matrix, which forbids the statement \( \Delta \geq 0 \iff \mathbf{W} \Delta \mathbf{W} \geq 0 \), about (89).