Semiclassical work and quantum work identities in Weyl representation

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Abstract
We derive a semiclassical nonequilibrium work identity by applying the Wigner–Weyl quantization scheme to the Jarzynski identity for a classical Hamiltonian. This allows us to extend the concept of work to the leading order in \( \hbar \). We propose a geometric interpretation of this semiclassical Jarzynski relation in terms of trajectories in a complex phase space and illustrate it with the exactly solvable case of the quantum harmonic oscillator.

Keywords: Jarzynski identity, semiclassics, Weyl quantization, quantum thermodynamics

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

According to the second principle of thermodynamics, macroscopic phenomena tend to evolve towards states corresponding to a maximum number of underlying microstates, i.e. states that maximize entropy. Combined with the first principle, this leads to a more operational statement for isothermal processes: the minimal amount of work to modify a system from a state \( A \) to a state \( B \) is given by

\[
W \geq F(B) - F(A),
\]

where \( F = U - TS \) is the free energy. Statistical mechanics has shown that the interpretation of macroscopic thermodynamics is statistical, by endowing microscopic states with a probability measure. Hence, the second principle should be understood as an average of a random process; one should write, in fact,

\[
\langle W \rangle \geq F(B) - F(A),
\]

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where \( \langle W \rangle \) is the average of path-dependent work along the realizations of a given macroscopic process (or protocol) leading from state \( A \) to state \( B \). In 1996, C. Jarzynski [1, 2] discovered that there exists a non-equilibrium work relation, underlying the long-established work inequality:

\[
\langle e^{-\beta W} \rangle = e^{-\beta (F(B) - F(A))}.
\]  

A remarkable consequence, from the thermodynamics point of view, is that, for (3) to be true, some individual realizations of the transform must ‘violate’ the second principle, that is, the system can reach once in a while a final state whose free energy variation is actually greater than the received work. The Jarzynski identity and its generalization by G. Crooks [3] have triggered an immense amount of work during the last two decades (see e.g. [4–6] for reviews) and has been verified experimentally [7–9].

The original approach of Jarzynski was based on classical trajectories and on the classical definition of work. It was therefore a challenge to generalize it to a quantum system. For closed quantum systems, this difficulty was overcome by the so-called two measurements process [10–17], where work is defined as the difference of energy between the end and the beginning of the evolution. This scheme was also studied using the Weyl formalism [18, 19] and path integrals [20]. As explained by Talkner et al [21], this definition of work does not correspond to a quantum observable because it cannot be represented by a Hermitian operator. This explains why alternative proposals based on some quantum work operator did not obey the Jarzynski identity [22–24]. For an open system, the two measurements scheme could be applied by considering the system together with its environment as a global, closed, system (see e.g. [25–27]). A different strategy to study open systems is to use a quantum map that acts on the density matrix of the system [28–30]. Under suitable assumptions, this map leads to a quantum Markov evolution, described by a Lindblad equation [31]. In this dynamical framework, a quantum analog of the Jarzynski relation can be proved by defining a work operator through a generalization of the Feynman–Kac formula to quantum Markov semi-groups (see [32] and references therein). Further studies and proposals for experimental checks of the quantum Jarzynski identity have unveiled the interplay between measurement, quantum trajectories and stochastic thermodynamics [33–46].

In [47], C. Jarzynski, H. T. Quan and S. Raav studied the semiclassical limit of the two measurements process to study the correspondence between the quantum and the classical definitions of work, and between the corresponding work distributions (see also [48, 49]). The aim of the present work is to revert the logic and to derive a quantum Jarzynski identity by using the Weyl representation of quantum mechanics. The advantage of this approach is to restore a classical phase space, allowing us, in the semiclassical regime, to define a pseudo-work along pseudo-trajectories, whose classical limit coincides with the definition traditional work along the classical trajectories. Our semiclassical definition of the work does not require the system to be closed and can be associated with a continuously measuring environment, such as modelled by Lindblad type equations, for which nonequilibrium work identities are valid [32].

The outline of this work is the following. In section 1, we review the basic properties of the Wigner–Weyl quantization scheme that will be used afterwards. In section 2, we consider a quantum system in thermal equilibrium at inverse temperature \( \beta \) governed by a time-independent Hamiltonian: starting from the Wigner transform of the density matrix, we define a 'pseudo-Hamiltonian' which, in the semiclassical limit, can be viewed as the average of the true classical Hamiltonian over a trajectory in complex time, of duration \( \Delta \tau = -i\hbar \beta \). In section 3, we study a system with a time-dependent Hamiltonian: we define a pseudo-work,
interpret it as the time-integral of the power generated by the pseudo-Hamiltonian over a complex trajectory and show that this pseudo-work satisfies semiclassical Jarzynski identity. This relation is illustrated by an explicit calculation for the harmonic oscillator in section 4. The last section is devoted to concluding remarks.

1. A brief review of Weyl quantization

In this section, we recall some basic properties of the Wigner–Weyl quantization scheme [50, 51] that we shall use in the present work. Elementary presentations can be found in [52–54] and more advanced discussions in [55, 56].

The Weyl transform allows us to construct an operator from a phase space function \( f(p, q) \). The idea is simply to take the Fourier transform of \( f \) and then to take a modified inverse Fourier transform, where the variables \( p \) and \( q \) are replaced by the operators \( \hat{p} \) and \( \hat{q} \). Literally, one has

\[
\hat{f} = \frac{1}{(2\pi \hbar)^2} \int \int e^{i\frac{k}{\hbar}(p\hat{p} + q\hat{q})} \left( \int \int f(\tilde{p}, \tilde{q})e^{-i\frac{k}{\hbar}(\tilde{p}\hat{p} + \tilde{q}\hat{q})} d\tilde{p} d\tilde{q} \right) dk_p dk_q. \tag{4}
\]

The integral gets simpler in the position representation, and, by applying Baker Campbell Hausdorff and the closure relation,

\[
e^{i\frac{k}{\hbar}(p\hat{p} + q\hat{q})} = e^{i\frac{k}{\hbar}\hat{q}\hat{q}} e^{i\frac{k}{\hbar}\hat{p}\hat{p}} e^{i\frac{k}{\hbar}\hat{q}\hat{q}} = \int e^{i\frac{k}{\hbar}\hat{q}\hat{q}} |p\rangle e^{i\frac{k}{\hbar}\hat{p}\hat{p}} \langle p| e^{i\frac{k}{\hbar}\hat{q}\hat{q}} \, dp, \tag{5}
\]

one ends up with

\[
\langle q' | \hat{f} | q'' \rangle = \frac{1}{2\pi \hbar} \int e^{i\frac{k}{\hbar}(q'-q'')} f \left( p, \frac{q' + q''}{2} \right) \, dp. \tag{6}
\]

This relation can be easily inverted, and, from any Hermitian operator \( \hat{A} \), one can define its ‘Weyl symbol’ \( \left[ \hat{A} \right]_W (p, q) \) by

\[
\left[ \hat{A} \right]_W (p, q) = \int e^{-i\frac{k}{\hbar}q} \left\langle q + \frac{Q}{2} | \hat{A} | q - \frac{Q}{2} \right\rangle dQ, \tag{7}
\]

which is a function of classical phase space. The Weyl symbol of a Hermitian operator is real, as can be seen easily by taking the complex conjugate of (7). This integral is sometimes called the Wigner transform. When the operator is a density operator, one adds a prefactor for normalization

\[
W(p, q) = \left[ \hat{A} \right]_W (p, q) = \frac{1}{2\pi \hbar} \int e^{-i\frac{k}{\hbar}q} \left\langle q + \frac{Q}{2} | \hat{A} | q - \frac{Q}{2} \right\rangle dQ. \tag{8}
\]

Since the transform is one-to-one, the Weyl representation is strictly equivalent to regular quantum mechanics. For operators made of a single variable, it actually respects the ‘correspondence principle’. For instance one has

\[
\left[ \hat{p}^n \right]_W (p, q) = p^n \]
\[
\left[ \hat{q}^n \right]_W (p, q) = q^n. \tag{9}
\]
On the other hand, the Weyl symbol of a product of non-commuting operators is generally not the product of the Weyl symbols of the operators. One has in fact

\[
\left[ \hat{A} \hat{B} \right]_W(p, q) = \frac{1}{\pi \hbar^2} \int e^{\frac{1}{\hbar} \left[ (p_1 - p)(q_2 - q) - (p_2 - p)(q_1 - q) \right]} A(p_1, q_1) B(p_2, q_2) \, dp_1 \, dq_1 \, dp_2 \, dq_2. \tag{10}
\]

For instance one has

\[
\left[ \hat{p} \hat{B} \right]_W(p, q) = \left( p + \frac{\hbar}{2i} \frac{\partial}{\partial q} \right) B(p, q)
\]
\[
\left[ \hat{q} \hat{p} \right]_W(p, q) = \left( q - \frac{\hbar}{2i} \frac{\partial}{\partial p} \right) \left( p + \frac{\hbar}{2i} \frac{\partial}{\partial q} \right) B(p, q). \tag{11}
\]

More generally, one has [53]

\[
\left[ \hat{A} \hat{B} \right]_W(p, q) = A \left( p + \frac{\hbar}{2i} \frac{\partial}{\partial q}, q - \frac{\hbar}{2i} \frac{\partial}{\partial p} \right) B(p, q). \tag{12}
\]

Although this product rule implies that products of operators are represented by complicated expressions, this simplifies in the case of symmetrized products of operators. For instance one has

\[
\left[ \hat{p} \hat{q} \right]_W(p, q) = pq + \frac{\hbar}{2i}
\]
\[
\left[ \hat{q} \hat{p} \right]_W(p, q) = pq - \frac{\hbar}{2i}
\]
\[
\left[ \frac{\hat{p} \hat{q} + \hat{q} \hat{p}}{2} \right]_W(p, q) = pq. \tag{13}
\]

This problem of ordering products disappears as soon as one takes the trace of a product of operators. Indeed, for every couple of operators \( \hat{A} \) and \( \hat{B} \) and their corresponding Weyl symbols \( A(p, q) \) and \( B(p, q) \), one has the following fundamental identity:

\[
\text{Tr} \, \hat{A} \hat{B} = \int \int A(p, q) B(p, q) \, dp \, dq. \tag{15}
\]

We emphasize that the Weyl symbol of a general function of a combination of non-commuting operators is generally not the function of the corresponding Weyl symbol:

\[
\left[ \exp \left( \hat{A} \right) \right]_W(p, q) \neq \exp \left( \left[ \hat{A} \right]_W(p, q) \right), \tag{16}
\]

(unless the operator \( A \) depends on a single variable, that is, \( \hat{A} = f(\hat{p}) \) or \( \hat{A} = f(\hat{q}) \)). In particular, this implies that one can not obtain a Jarzynski equality in the Weyl representation by simply quantizing the classical Jarzynski proof, which is based on the properties of the exponential function. One of the motivations of the present work is to overcome this difficulty (see in section 3).
2. Semiclassical approximation of a thermal state

In this section, we construct in the classical phase space a ‘pseudo-Hamiltonian’ \( \Gamma(p, q) \), defined from the Weyl symbol of the thermal state generated by the quantum Hamiltonian \( \hat{H} \). The function \( \Gamma(p, q) \) is defined in the following way:

\[
\left[ e^{-\beta \hat{H}} \right]_w (p, q) \equiv e^{-\beta \Gamma(p, q)},
\]

(17)

we emphasize again that, because of (16), we have \( \Gamma(p, q) \neq H(p, q) \), where \( H(p, q) \) is the classical Hamiltonian. The exact formula \( \Gamma \) is rather complicated but we can derive an approximate expression \( G(p, q) \propto \Gamma(p, q) \) in the semiclassical limit, by interpreting the thermal state as a Schrödinger propagator during an imaginary time \([57, 58]\)

\[
e^{-\beta \hat{H}} = e^{-\frac{\beta}{\hbar} \Delta \tau \hat{H}},
\]

(18)

where

\[
\Delta \tau = -i \hbar \beta
\]

(19)

is interpreted as an imaginary time. For a real \( \Delta \tau \), this propagator can be well approximated by the Van Vleck propagator \([59]\), which plugged into (8), gives the semiclassical Wigner propagator calculated by M V Berry (see equation (21) of \([60]\)). Therefore, using Berry’s result, the semiclassical Wigner thermal state is simply the continuation of this propagator for imaginary \( \Delta \tau \).

In this section, we rederive the expression of the semiclassical Wigner thermal state by the stationary phase method. This will allow us to introduce notations and techniques that will be useful in the rest of this work. Starting from equation (38.30) of \([59]\), we write

\[
\langle q_i \mid e^{-\frac{i}{\hbar} \beta (q_i - q_f)} \mid q_f \rangle \simeq K_c(q_i, t_i; q_f, t_f) \equiv \sum_j \frac{1}{(2\pi \hbar)^{3/2}} \left| \frac{\partial p_j}{\partial q_j} \right|^{1/2} e^{\frac{i}{\hbar} \beta S_j(q_i, t_i; q_f, t_f) - \frac{i}{\hbar} \beta \int_{t_i}^{t_f} \beta S_j(q_i, t_f) dt_f},
\]

(20)

where \( S_j \) is a solution of a Hamilton–Jacobi equation or its time reverse,

\[
\frac{\partial S_j}{\partial t_f} + H \left( \frac{\partial S_j}{\partial q_f}, q_f \right) = 0, \quad \frac{\partial S_j}{\partial t_i} - H \left( -\frac{\partial S_j}{\partial q_i}, q_i \right) = 0,
\]

(21)

and coincides with the classical action calculated along one of the jth classical trajectories \( (p_j(t), q_j(t)) \) generated by \( H(p, q) \), the classical counterpart of \( \hat{H} \), such that

\[
\begin{align*}
q_j(t_i) &= q_i, \\
q_j(t_f) &= q_f,
\end{align*}
\]

\[
\left\{ \begin{array}{ll}
\partial_t p_j(t) &= -\partial_q H (p_j(t), q_j(t)) \\
\partial_t q_j(t) &= \partial_p H (p_j(t), q_j(t)),
\end{array} \right.
\]

There are a priori several classical trajectories, labelled by \( j \), and the propagator (20) sums over all the trajectories having the right initial and final conditions. The integers \( m_j \) in equation (20) are the Maslov indices, which count the number of times the \( j \)th trajectory crosses a caustic, that is, the set of points where \( \frac{\partial p_j}{\partial t_i} \) is singular \([59, 61]\). These caustics are reached only after a
certain amount of time; before that time, there is a unique trajectory for two given boundary conditions, here \((q_i, t_i)\) and \((q_f, t_f)\). Thus, we have

\[
S(q_i, t_i; q_f, t_f) = \int_{t_i}^{t_f} \left[ p(t) \partial_t q(t) - H(p(t), q(t)) \right] dt \\
= \int_{t_i}^{t_f} p(t) \delta q(t) dt - (t_f - t_i) H(p(t_i), q(t_i)),
\]

the last line being true only for a time independent Hamiltonian. We also have, from the fact that \(S\) is solution of (21), and see chapter 46 of [62] for the whole story,

\[
\begin{aligned}
\frac{\partial S}{\partial q_i} &= -p_i \\
\frac{\partial S}{\partial t_i} &= H(p_i, q_i) \\
\frac{\partial S}{\partial q_f} &= p_f \\
\frac{\partial S}{\partial t_f} &= -H(p_f, q_f).
\end{aligned}
\]

We now take the analytical continuation of this propagator and obtain

\[
\langle q_f | e^{-i\hat{H}} | q_i \rangle \simeq K_{sc}(q_i, \tau_i; q_f, \tau_f) \\
\simeq \frac{1}{(2\pi\hbar)^{1/2}} \left| \frac{\partial^2 S}{\partial q_f \partial q_i} \right|^{1/2} e^{iS(q_i, \tau_i; q_f, \tau_f)},
\]

with \(\tau_i \in i\mathbb{R}\) and \(\tau_f = \tau_i + \Delta \tau \in i\mathbb{R}\) purely imaginary times. We have supposed that all Maslov indices \(m_i\) vanish: this requires the imaginary time to be small enough to avoid the first caustics of the complex trajectory. Like in regular WKB method, the caustics corresponds to the singularities of the second derivative of the Jacobian of \(S\), and the Maslov indices increase by one every time the trajectory crosses a caustic. It is a consequence of the necessary change of representation, from \((p, q)\) to the Fourier conjugate variables \((\xi_p, \xi_q)\), in order to have a non singular expression of the propagator in the neighbourhood of the caustic. This procedure is more delicate in the complex domain than in the real one, as one needs to chose the ‘correct branch’ connecting the trajectory from both sides of the caustic. This is the Stokes phenomenon.

To obtain a correct ordering of the \(h\) corrections, the value of \(\Delta \tau = \tau_f - \tau_i\) must remain constant as \(h \to 0\) [63]. This corresponds to a semiclassical regime at low temperature (large \(\beta\)). Although the limit itself, \(h = 0\), cannot really be interpreted as a classical regime, since it must occur at 0 temperature which is the realm of quantum regime, we can expect that finite values of \(h\) and finite values of temperature can be in this intermediate regime. We remark that the initial imaginary ‘time’ \(\tau_i \in i\mathbb{R}\) is, a priori, a free parameter, since the Hamiltonian is not a function of \(\beta\). Let us now have a closer look at the action \(S\): we consider the imaginary time classical trajectory \((p(\tau), q(\tau))\) generated by \(H(p, q)\), such that

\[
\begin{aligned}
q(\tau_i) &= q_i \\
\partial_\tau p(\tau) &= -\partial_q H(p(\tau), q(\tau)) \\
\partial_\tau q(\tau) &= \partial_p H(p(\tau), q(\tau)),
\end{aligned}
\]

\[
\begin{aligned}
q(\tau_f) &= q_f \\
\partial_\tau p(\tau) &= -\partial_q H(p(\tau), q(\tau)) \\
\partial_\tau q(\tau) &= \partial_p H(p(\tau), q(\tau)),
\end{aligned}
\]
where $\tau$ is an imaginary parameter with $\tau \in [\tau_i, \tau_f]$. This trajectory is generically unique and the action $S$ (which is now imaginary) is calculated by integrating along this trajectory (26),

$$S(q_i, \tau_i; q_f, \tau_f) = \int_{\tau_i}^{\tau_f} \left[ p(\tau) \partial_\tau q(\tau) - H(p(\tau), q(\tau)) \right] d\tau$$

$$= \int_{\tau_i}^{\tau_f} p(\tau) \partial_\tau q(\tau) d\tau - \Delta \tau H(p(\tau_i), q(\tau_i)).$$

(27)

We now evaluate (17) by plugging the semiclassical expression (25) in the Wigner transform (8):

$$\left[ e^{-i\hat{H}} \right]_w (p, q) = \frac{1}{2\pi \hbar} \int e^{\frac{i}{\hbar}pQ} \left\langle q + \frac{Q}{2} \right| e^{-i\hat{H}} \left| q - \frac{Q}{2} \right\rangle dQ$$

$$\simeq \frac{1}{2\pi \hbar} \int \frac{1}{(2\pi \hbar)^{1/2}} \left| \frac{\partial^2 S}{\partial q_i \partial q_f} \right|^{1/2} e^{\frac{i}{\hbar}S_{tot}(p, q, Q)} dQ.$$  

(28)

for every $Q$, the total action

$$S_{tot}(p, q, Q) = -pQ + \left[ q - \frac{Q}{2}, \tau_i; q + \frac{Q}{2}, \tau_f \right],$$

(29)

defines, implicitly, a classical trajectory $(p_i, q_i) \rightarrow (p_f, q_f)$ such that

$$q_i = q(\tau_i) = q - \frac{Q}{2}$$

$$q_f = q(\tau_f) = q + \frac{Q}{2}.$$  

(30)

In the semiclassical limit, $\hbar \rightarrow 0$, keeping $\Delta \tau$ fixed, the stationary phase method can be used; the main contribution in the integral (28) is given by the stationary point $Q^*$, that solves

$$\frac{\partial}{\partial Q} S_{tot}(p, q, Q)|_{Q^*} = -\frac{1}{2} \frac{\partial S}{\partial q_i} \left( q - \frac{Q^*}{2}, \tau_i; q + \frac{Q^*}{2}, \tau_f \right)$$

$$+ \frac{1}{2} \frac{\partial S}{\partial q_f} \left( q - \frac{Q^*}{2}, \tau_i; q + \frac{Q^*}{2}, \tau_f \right) - p = 0.$$  

(31)

Thus, according to (24), we obtain

$$p = \frac{p_i + p_f}{2}.\quad (32)$$

Using equations (30) and (32), we then conclude that among the family of trajectories $(p(\tau), q(\tau))$ spanned by $Q$, we must select the stationary trajectory $(p^*(\tau), q^*(\tau))$ such that

$$\frac{p_i^* + p_f^*}{2} = p\quad (33)$$

$$\frac{q_i^* + q_f^*}{2} = q.\quad (34)$$
where \((p_i^*, q_i^*) = (p^*(\tau), q^*(\tau))\) and \((p_i^+, q_i^+) = (p^*(\tau), q^*(\tau))\). To understand the structure of the solution, let us define the imaginary time flow \((p', q') \mapsto (p(\tau), q(\tau)) = C_{\tau}(p', q')\) with \((p(\tau), q(\tau))\) solution of equation (26) and \((p(0), q(0)) = (p', q')\). Formally, one can write

\[
\begin{align*}
p(\tau) &= p(0) + \tau \dot{p}(0) + \frac{1}{2} \tau^2 \ddot{p}(0) + \ldots \\
q(\tau) &= q(0) + \tau \dot{q}(0) + \frac{1}{2} \tau^2 \ddot{q}(0) + \ldots
\end{align*}
\]

(35)

We first note that, for real \((p(0), q(0))\), then \(\dot{p}(0), \ddot{p}(0)\ldots\) are also real, as they can be obtained from (22) and expressed in terms of derivatives of the type \(\partial_{p, q} H(p(0), q(0))\) where \(H\) is real. On the other hand, \(\tau\) is imaginary. Therefore one then has, for real \((p', q')\),

\[
C_{\tau}(p', q') = C_{-\tau}(p', q').
\]

(36)

Let us then build the map

\[
(p', q') \mapsto \mathcal{M_{\Delta^\tau}}(p', q') = \frac{C_{\Delta^\tau}(p', q') + C_{\Delta^\tau}(q', p')}{2}.
\]

(37)

From (36), \(\mathcal{M_{\Delta^\tau}}\) is a real map from the real phase space \(\{(p', q')\}\) to itself. Then, we define

\[
(p', q') = \left(\mathcal{M_{\Delta^\tau}}\right)^{-1}(p, q).
\]

(38)

Obviously,

\[
\begin{align*}
(p_i^*, q_i^*) &= C_{\Delta^\tau}(p_i^*, q_i^*) \\
(p_i^+, q_i^+) &= C_{\Delta^\tau}(p_i^+, q_i^+)
\end{align*}
\]

(39)

then fulfill conditions (33) and (34). This construction makes it clear that

\[
\begin{align*}
p_i^* &= p_i^+ \\
q_i^* &= q_i^+
\end{align*}
\]

(40)

which implies, from equation (30) with \(q\) being real, that \(q_i^\ast\) is in fact the imaginary part of \(q_i\), with

\[
Q^\ast = -Q^*.
\]

(41)

To summarize, the arc \((p^*(\tau), q^*(\tau))\) is symmetric with regard to the real phase space plane, and it intersects this real phase space plane at \((p_i^*, q_i^*) = (p^* \left(\frac{\Delta^\tau}{\Delta^\tau}\right), q^* \left(\frac{\Delta^\tau}{\Delta^\tau}\right))\). Moreover, the chord \((p_i^* - p_i^+ , Q^*)\) of this arc is purely imaginary, and the middle of this chord is \((p, q)\). The picture is shown on figure 1. Finally, we retrieve for the Weyl symbol, defined in (28), an expression equivalent to the one in [60], but in imaginary time, that is

\[
\left[e^{\frac{-i\Gamma}{\hbar}}\right]_W(p, q) = e^{\frac{-i\Gamma(p, q)}{\hbar}} \simeq \mathcal{N}(p, q) e^{\frac{-iG(p, q)}{\hbar}}
\]

(42)
with
\[ G(p, q) = -\frac{1}{\Delta \tau} \left[ -pQ^* + S \left( q - \frac{Q^*}{2}, \tau; q + \frac{Q^*}{2}, \tau \right) \right] \]
\[ = H (p^*_c, q^*_c) - \frac{1}{\Delta \tau} \left[ \int_{\tau_i}^{\pi} p^*(\tau) \partial_\tau q^*(\tau) d\tau - pQ^* \right] \]
\[ = H (p^*_c, q^*_c) - \frac{1}{\Delta \tau} A(p, q) \] (43)

and the prefactor
\[ \mathcal{N}(p, q) = \frac{1}{2\pi \hbar} \frac{1}{2(\pi \hbar)^{1/2}} \frac{\partial^2 S^*}{\partial q \partial q_1}^{1/2} \mathcal{F} \sqrt{\frac{\pi}{\hbar}} \mathcal{S}_{\text{tot}}(Q^*) \]
\[ = \frac{1}{2\pi \hbar} \frac{1}{2(\pi \hbar)^{1/2}} \frac{\partial^2 S^*}{\partial q \partial q_1}^{1/2} e^{i\frac{\pi}{4}} \sqrt{\frac{1}{\hbar}} \mathcal{S}_{\text{tot}}(Q^*) \]
\[ = \frac{1}{2\pi \hbar} \sqrt{\frac{\partial^2 S^*}{\partial q \partial q_1} - \frac{1}{2} \left( \frac{\partial^2 S^*}{\partial q^2} + \frac{\partial^2 S^*}{\partial q_1^2} \right)} \] (44)

Here, \( S^* \) represents the action \( S \) evaluated at the saddle-point. The term \( A(p, q) = i \int_{\tau_i}^{\pi} p^*(\tau) \partial_\tau q^*(\tau) d\tau - i pQ^* \) is a real number that can be interpreted as the area between the complex arc \( (p^*(\tau), q^*(\tau)) \) and its chord, as shown in figure 1. As a consequence, \( G(p, q) \) is also a real function. On the other hand, \( \Gamma(p, q) \) is also real since the Weyl representation of any Hermitian operator is real, as can easily be checked from (7). The prefactor (44) is the product of two terms: one arises from the Van Vleck propagator and the other is generated by the stationary phase method (i.e. an imaginary Gaussian integration). In the following, we shall keep the leading order in \( \hbar \) only and the prefactor \( \mathcal{N}(p, q) \) will be omitted.

3. A Jarzynski identity in the Weyl representation

In the previous section, using a semiclassical approach, we have derived an expression for the function \( G(p, q) \) such that \( e^{-\Delta \mathcal{F}(p, q)} \) represents the quantum thermal state generated by the (quantum) Hamiltonian \( \hat{H} \). We shall now introduce an explicit time dependence in the Hamiltonian \( H_t \), define a pseudo-work, calculate its semiclassical expression \( \partial_t G_t \), and derive a formal Jarzynski identity. The heart of the matter resides in the geometric interpretation of the semiclassical trajectories.

3.1. Time-dependent Hamiltonian

We use the semiclassical scheme constructed in section 2, but with a time dependent Hamiltonian \( H_t(p, q) \). In this context, it is important to be aware that the 'imaginary time' \( \tau \) of the
Figure 1. The complex trajectory crosses the real plane at \((p^c, q^c)\); its chord \((p^r - p^c, Q^r)\) is imaginary and the middle of this chord is \((p, q)\). Also, \((p, q)\) is the image of \((p^c, q^c)\) through \(M_{\Delta \tau}^2\).

trajectory (26), which is related to the temperature \(1/\beta\), has nothing to do with the physical time \(t\). In particular, the physical time \(t\) must remain frozen during the imaginary time propagation in (26). In other words, the imaginary time trajectory \((p_t(\tau), q_t(\tau))\) obeys

\[
\begin{align*}
q(\tau_i) &= q_i, \\
q(\tau_f) &= q_f \\
\partial_{\tau} p(\tau) &= -\partial_q H_t(p(\tau), q(\tau)) \\
\partial_{\tau} q(\tau) &= \partial_p H_t(p(\tau), q(\tau)),
\end{align*}
\]

(45)

with a fixed value of \(t\). This also means that \(S^*\) and \(Q^*\) and \((p^*(\tau), q^*(\tau))\) are then functions of \(t\).

Remark: We emphasize that the trajectory (45) is not the analytical continuation of the real trajectory generated by \(H_t(p, q)\). Indeed, such a continuation \((\bar{p}(\tau), \bar{q}(\tau))\) would obey a slightly different equation

\[
\begin{align*}
\bar{q}(\tau_i) &= q_i, \\
\bar{q}(\tau_f) &= q_f \\
\partial_{\tau} \bar{p}(\tau) &= -\partial_{\bar{q}} H_t(p(\tau), q(\tau)) \\
\partial_{\tau} \bar{q}(\tau) &= \partial_{\bar{p}} H_t(p(\tau), q(\tau)),
\end{align*}
\]

(46)

Here, the Hamiltonian is changing along the trajectory.

For any given value of \(t\), we calculate \(G_t(p, q)\), the Van Vleck approximation of the pseudo-Hamiltonian log \(\left[ e^{-\beta H_t} \right] \_W (p, q)\), by using equation (43).

We now define the pseudo-work as \(\partial_t G_t(p, q)\). The expression of this time derivative is actually simpler than the expression of \(G_t(p, q)\) itself, as we shall now show. We first consider the time-dependent stationary phase trajectory, \((p_t^* (\tau), q_t^* (\tau))\). Using equation (29), we write

\[-\Delta \tau G_t(p, q) = S_{\text{w}}(p, q, Q^*, t) = -p Q^* + S_t^c \left( q - \frac{Q^*}{2} \tau_i; q + \frac{Q^*}{2} \tau_f \right),\]

(47)
where $Q^*$ is a function of time $t$. Taking derivative with respect to time, we obtain after using (31):

$$-\Delta \tau \partial_t G_i(p, q) = \frac{\partial}{\partial t} S_{\text{tot}}(p, q, Q^*, t) + \frac{\partial}{\partial Q^*} S_{\text{tot}}(p, q, Q^*, t) \frac{\partial Q^*}{\partial t}$$

$$= \frac{\partial}{\partial t} S_{\text{tot}}(p, q, Q^*, t)$$

$$= \frac{\partial}{\partial t} S_i^* \left( q - \frac{Q^*}{2}, \tau; q + \frac{Q^*}{2}, \tau \right)$$

$$= \lim_{\Delta \tau \to 0} \frac{d}{dt} \left( S_{\text{tot}}^* \left( q - \frac{Q^*}{2}, \tau; q + \frac{Q^*}{2}, \tau \right) - S_i^* \left( q - \frac{Q^*}{2}, \tau; q + \frac{Q^*}{2}, \tau \right) \right).$$

(48)

We made explicit the latter time derivative so that the reader can remind that $S_{\text{tot}}^*$ and $S_i^*$ actually live on two different stationary phase trajectories, with an implicit $t$ dependence. However, the trajectory for time $t + \Delta \tau$ can be seen as a fluctuation $(p(\tau) + \delta p(\tau), q(\tau) + \delta q(\tau))$ around the trajectory $(p(\tau), q(\tau))$ for time $t$, therefore,

$$-\Delta \tau \partial_t G_i(p, q) = \lim_{\Delta \tau \to 0} \frac{1}{\Delta \tau} \int_{\tau}^{\tau + \Delta \tau} \left[ (p(\tau) + \delta p(\tau)) \partial_t (q(\tau) + \delta q(\tau)) - H_{\tau+\Delta \tau} (p(\tau) + \delta p(\tau), q(\tau)) \right.$$

$$+ \delta q(\tau) - p(\tau) \partial_t q(\tau) + H_{\tau} (p(\tau), q(\tau))] \, d\tau,$$

(49)

and, because of the stationarity of the action around $(p(\tau), q(\tau))$ with the same initial and final positions and times, the first order terms in $(\delta p(\tau), \delta q(\tau))$ cancels out, and only remains the derivative with respect to the explicit time dependence of $H$, therefore

$$\partial_t G_i(p, q) = \frac{1}{\Delta \tau} \int_{\tau}^{\tau + \Delta \tau} \partial_t H_i \left( p_i^*(\tau), q_i^*(\tau) \right) \, d\tau.$$  

(50)

To summarize, we have shown that in the semiclassical limit $e^{-\beta H_i}$ can be approximately represented by a function $e^{-\beta G_i(p, q)}$ in the Weyl space and that the associated work $\partial_t G_i(p, q)$ is given by a simple expression as an average of $\partial_t H_i(p, q)$ over a complex trajectory.

We note that

$$\lim_{\hbar \to 0} G_i(p, q) \neq H_i(p, q),$$

(51)

because, when $\Delta \tau$ is fixed, the $\hbar \to 0$ limit has to be taken together with $\beta \to +\infty$: this is not a classical limit. On the other hand, we do have

$$\lim_{\Delta \tau \to 0} G_i(p, q) = H_i(p, q),$$

(52)

In order to have all the ingredients to build a quantum identity which resembles formally to a Jarzynski identity, we need trajectories in the Weyl space (along which the pseudo-work is integrated). We now explain how to construct these trajectories with the help of techniques developed in [64].
3.2. Trajectories in Weyl space

A key ingredient of the Jarzynski identity [1, 2] is the power $\partial_t \mathcal{H}(p(t), q(t))$ along a classical trajectory $(p(t), q(t))$, whose integral over $t$ gives the work. The exponential of the Jarzynski work relates the initial distribution $\Pi_0(p, q) = e^{-\beta \mathcal{H}(p, q)}$ to the distribution at the final time $\Pi_f(p(t), q(t))$ defined as

$$\Pi_i(p(t), q(t)) = e^{-\beta \mathcal{H}(p(t), q(t))}$$

where $(p(t), q(t))$ is the image under the Hamiltonian flow of the initial point $(p(0), q(0)) = (p, q)$ in the phase space. Now, if $\hat{\Pi}_i = e^{-\beta \hat{H}_t}$ is the, not normalized, quantum thermal operator, and if the Weyl symbol of $\hat{\Pi}_i$ is $e^{\gamma(p,q)}$, from equation (17), we would like to translate $\Pi_i(p(t), q(t))$ as a kind of propagation of $e^{\gamma(p,q)}$ in phase space.

We can first remark that $\Gamma_i(p, q)$ considered as a Hamiltonian, can generate trajectories $(p_t(t), q_t(t))$ in phase space. Then, $e^{\gamma(p_t(q_0), q(t))}$ could serve as a backbone for a Jarzynski equality in the Weyl representation, by formally reproducing the initial Jarzynski proof as if $\Gamma_t(p, q)$ was a classical Hamiltonian (see appendix A). However this formal dynamics in phase space has no connection with the quantum evolution, which seems desirable if we want to obtain a quantum Jarzynski identity with physical meaning. For this reason, in order to find a satisfactory translation of $\Pi_i(p(t), q(t))$ in the Weyl representation, we will focus on the fact that it is simply the Liouville propagation of the classical distribution $\Pi_i(p, q)$, that is

$$\frac{d}{dt} (\Pi_i(p(t), q(t))) = \partial_t \Pi_i(p(t), q(t)) + \partial_p \Pi_i(p(t), q(t)) \partial_t p(t) + \partial_q \Pi_i(p(t), q(t)) \partial_t q(t)$$

$$= \partial_t \Pi_i(p(t), q(t)) - \partial_t \Pi_i(p(t), q(t)) \partial_t H_t(p(t), q(t))$$

$$+ \partial_q \Pi_i(p(t), q(t)) \partial_t H_t(p(t), q(t))$$

$$= \partial_t \Pi_i(p(t), q(t)) - \{H_t, \Pi_i\}(p(t), q(t)). \tag{53}$$

This Liouville propagation will then be translated into the quantum unitary propagation $\hat{U}_i^\dagger \hat{\Pi}_i \hat{U}_i$ of $\Pi_i$, and we shall use the fact that any quantum evolution in the Weyl representation can be described, in the semiclassical limit, as a generalized Liouville propagation, see [64]. We can find indeed a trajectory $(\hat{p}(t), \hat{q}(t))$ in phase space, such that

$$\left[ \hat{U}_i^\dagger \hat{\Pi}_i \hat{U}_i \right]_W (p, q) \simeq \left[ \hat{A} \right]_W (p(t), q(t)) \tag{54}$$

where $(\hat{p}(t), \hat{q}(t))$ tends to the classical trajectory $(p(t), q(t))$ when $\hbar \to 0$. To resume, the solution $\Pi_i(p(t), q(t))$ of (53) will be mapped to $e^{\gamma(p(t), q(t))}$, which is the approximate Weyl representation of $\hat{U}_i^\dagger \hat{\Pi}_i \hat{U}_i$, solution of

$$\frac{d}{dt} \left( \hat{U}_i^\dagger \hat{\Pi}_i \hat{U}_i \right) = \hat{U}_i^\dagger \left( \partial_t \hat{\Pi}_i \right) \hat{U}_i - \hat{U}_i^\dagger \frac{1}{\hbar} \left[ \hat{H}_t, \hat{\Pi}_i \right] \hat{U}_i. \tag{55}$$

This path $(\hat{p}(t), \hat{q}(t))$ is defined as in [64], the difference being that $e^{\gamma(p(t), q(t))}$ is interpreted as an imaginary time propagator. The original construction of [64] is thus shifted into the complex domain, and $(\hat{p}(t), \hat{q}(t))$ appears as the middle curve of two complex (nonreal) classical trajectories.
We begin with the Weyl symbol of $\hat{U}(t_0, T) e^{-i\beta T} \hat{U}(t_0, T)$. Once again we use the matrix element (20) into the Weyl transform (7), in real time for the real propagation, and in imaginary time for the temperature propagation,

$$
\left[ \hat{U}(t_0, T) e^{-i\beta T} \hat{U}(t_0, T) \right]_w(p, q) = e^{\frac{iQp}{\hbar}} \left\langle q + \frac{Q}{2} \bigg| \hat{U}(t_0, T) e^{-i\beta T} \hat{U}(t_0, T) \bigg| q - \frac{Q}{2} \right\rangle \, dQ
$$

$$
= \iiint e^{\frac{iQp}{\hbar}} \left\langle q + \frac{Q}{2} \bigg| \hat{U}(t_0, T) \right| q + \frac{Q}{2} \rangle \, dQ \langle q_1 | e^{-i\beta T} | q_2 \rangle \langle q_2 | \hat{U}(t_0, T) \bigg| q - \frac{Q}{2} \rangle \, dQ \, dq_1 \, dq_2
$$

$$
\approx \iiint e^{\frac{iQp}{\hbar}} \langle q_1 \big| \hat{U}(t_0, T) \big| q_2 \rangle \, dQ \, dq_1 \, dq_2,
$$

(56)

where $\tau$ is the complex conjugate of $\zeta$, and the total action $S_{tot}$ is now

$$
S_{tot}(p, q, Q, q_1, q_2, t_0, T) = -pQ - S_- \left( q + \frac{Q}{2}, t_0, q_1, T \right) + S_T(q_2, \tau; q_1; \tau) + S_+ \left( q - \frac{Q}{2}, t_0, q_2, T \right),
$$

(57)

with $\tau = \tau_1 + \Delta \tau \in i\mathbb{R}$. Hence the total action is made of the real time action $S_+$ counting positively, the complex time action $S_T$ and the real time action $S_-$ counted negatively. We warn the reader again that the complex time action is not the analytical continuations of the real time ones, as already mentioned in section 3.1.

The action $S_+(q - \frac{Q}{2}, t_0; q_2, T) = \int_{t_0}^{T} \left[ p_+(t) \partial t q_+(t) - H_t(p_+(t), q_+(t)) \right] dt$ is calculated along a regular classical trajectory $(p_+(t), q_+(t))$, generated by $H_t(p, q)$ with running $t$, that is,

$$
\begin{cases}
q_+(t_0) = q - \frac{Q}{2} \\
q_+(T) = q_2 \\
p_+(t) = -\partial_t H_t(p_+(t), q_+(t)) \\
q_+(t) = \partial_t H_t(p_+(t), q_+(t))
\end{cases}
$$

(58)

the action $S_T(q_2, \tau_1; q_1, \tau_1) = \int_{\tau_1}^{\tau_1} \left[ p_2(\tau) \partial_\tau q_2(\tau) - H_T(p_2(\tau), q_2(\tau)) \right] d\tau$, is calculated along the classical trajectory $\tau \mapsto (p_2(\tau), q_2(\tau))$ generated by $H_t(p, q)$, in which the time dependence $T$ has been frozen. More explicitly, we have

$$
\begin{cases}
q_2(\tau_1) = q_2 \\
p_2(\tau_1) = -\partial_\tau H_T(p_2(\tau), q_2(\tau)) \\
q_2(\tau) = \partial_\tau H_T(p_2(\tau), q_2(\tau))
\end{cases}
$$

(59)

where $\tau$ is imaginary. Finally, $S_-(q_1, t_0; q + \frac{Q}{2}, T) = \int_{t_0}^{T} \left[ p_-(t) \partial t q_-(t) - H_t(p_-(t), q_-(t)) \right] dt$, is calculated along a regular classical trajectory $(p_-(t), q_-(t))$, generated by $H_t(p, q)$ with running $t$, that is,

$$
\begin{cases}
q_-(t_0) = q + \frac{Q}{2} \\
q_-(T) = q_1 \\
p_-(t) = -\partial_t H_t(p_-(t), q_-(t)) \\
q_-(t) = \partial_t H_t(p_-(t), q_-(t))
\end{cases}
$$

(60)
Notice that $-S_-\left( q + \frac{Q}{2}, t_0; q_1, T \right)$ can be interpreted both as the opposite of an action with forward trajectory, describing the matrix element $\langle q_1 | \hat{U}(t_0, T) | q + \frac{Q}{2} \rangle$; and as a positive action along a backward trajectory, $-S_-\left( q + \frac{Q}{2}, t_0; q_1, T \right) = S_-\left( q_1, t_0; q + \frac{Q}{2}, T \right)$, describing the matrix element $\langle q + \frac{Q}{2} | \hat{U}(t_0, T)^\dagger | q_1 \rangle$. We found that the former way makes calculations easier to follow.

We evaluate now expression (56) with stationary phase method, that is, we replace the integral over $Q, q_1, q_2$ by a single value of the integrand at the generically unique triple $(Q^*, q_1^*, q_2^*)$ such that

$$\frac{\partial}{\partial Q} S_{\text{tot}}(p, q, Q^*, q_1^*, q_2^*, t_0, T) = -\frac{1}{2} \partial_{q_1} S_-\left( q + \frac{Q^*}{2}, t_0; q_1^*, T \right) - \frac{1}{2} \partial_{q_2} S_+\left( q - \frac{Q^*}{2}, t_0; q_2^*, T \right) - p = 0$$

(61)

$$\frac{\partial}{\partial q_1} S_{\text{tot}}(p, q, Q^*, q_1^*, q_2^*, t_0, T) = \partial_{q_1} S_T\left( q_1^*, \tau; q_1^*, \tau \right) + \partial_{q_2} S_+\left( q + \frac{Q^*}{2}, t_0; q_2^*, T \right) = 0$$

(62)

$$\frac{\partial}{\partial q_2} S_{\text{tot}}(p, q, Q^*, q_1^*, q_2^*, t_0, T) = -\partial_{q_2} S_-\left( q + \frac{Q^*}{2}, t_0; q_1^*, T \right) + \partial_{q_2} S_T\left( q_2^*, \tau; q_1^*, \tau \right) = 0$$

(63)

This defines three trajectories,

1. $(p_+^*(t), q_+^*(t))$, associated with $S_+\left( q - \frac{Q^*}{2}, t_0; q_2^*, T \right)$, solution of (58) with $q_+^*(t_0) = q - \frac{Q^*}{2}$ and $q_+^*(T) = q_2^*$,
2. $(p_+^*(\tau), q_+^*(\tau))$, associated with $S_T\left( q_2^*, \tau; q_1^*, \tau \right)$, solution of (59) with $q_+^*(\tau) = q_2^*$ and $q_+^*(\tau) = q_1^*$,
3. $(p_-^*(t), q_-^*(t))$, associated with $S_-\left( q + \frac{Q^*}{2}, t_0; q_1^*, T \right)$, solution of (60) with $q_-^*(T) = q_1^*$ and $q_-^*(t_0) = q + \frac{Q^*}{2}$,

such that, according to equation (61), and using (24), we have

$$\frac{p_+^*(t_0) + p_+^*(t_0)}{2} = p$$

and

$$\frac{q_+^*(t_0) + q_+^*(t_0)}{2} = q + \frac{Q^*}{2} + q - \frac{Q^*}{2} = q.$$  

(64)

Then, from equation (62) with (24), we obtain

$$p_+^*(T) = p_+^*(\tau)$$

$$q_+^*(T) = q_+^*(\tau) = q_2^*.$$  

(65)

and equation (63) with (24) imply

$$p_-^*(T) = p_-^*(\tau)$$

$$q_-^*(T) = q_-^*(\tau) = q_1^*.$$  

(66)

To construct this set of three trajectories, one proceed as in the time independent case. We define the complex time propagator $C^0[p']$ such that

$$C_0^{(p', q')} = (p', q') \quad \partial_t C_0^{(p', q')} = \mathcal{J} \nabla H, \quad C^0[(p', q')] = J.$$  

(67)
with $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and the real time classical propagator $R_{\tau, t}$, such that

$$R_{\tau, t}(p', q') = (p', q') \quad \partial_t R_{\tau, t}(p', q') = J \nabla H_t \left( R_{\tau, t}(p', q') \right).$$

We already saw in equation (36) of section 2 that, for real $(p', q')$, the positive imaginary time propagation is the complex conjugate of the negative imaginary time propagation, that is,

$$C^{[i]}(p', q') = \overline{C^{[i]}(p', q')}.$$  

(69)

On the other hand, for any complex $(p'', q'')$, one has

$$R_{\tau, t}(p'', q'') = R_{\tau, t}(p'', q''),$$

(70)

since the Hamiltonian $H_t$ and times $t$ and $\tau$ are real, that is, the real time propagation conserves the complex conjugate relation between two phase space points. As a consequence, the map $M_{\tau, t}$, defined by

$$(p', q') \mapsto M_{\tau, t}(p', q') = \frac{(R_{\tau, t})^{-1} \left( C^{[i]}(p', q') \right) + (R_{\tau, t})^{-1} \left( C^{[i]}(p', q') \right)}{2},$$

(71)

is a real map, that is, it maps the real phase space $\{(p', q') \in \mathbb{R}^2\}$ to itself. It is then easy to define the inverse image $(p'_\tau, q'_\tau)$ of $(p, q)$ through map $M_{\tau, t}$, that is

$$(p'_\tau, q'_\tau) = \left( M_{\tau, t} \right)^{-1}(p, q),$$

(72)

and, from this point, to define the whole stationary phase trajectory. One has indeed,

$$(p^T_\tau(\tau), q^T_\tau(\tau)) = C^{[i]}(p^\tau, q^\tau),$$

$$(p^T_\tau(\tau), q^T_\tau(\tau)) = C^{[i]}(p^\tau, q^\tau),$$

$$(p^T_\tau(t), q^T_\tau(t)) = (R_{\tau, t})^{-1}(p^T_\tau(\tau), q^T_\tau(\tau)),$$

$$(p^T_\tau(t), q^T_\tau(t)) = (R_{\tau, t})^{-1}(p^T_\tau(\tau), q^T_\tau(\tau)).$$

(73)

The picture is represented on figure 2.

Notice that, $q^T_\tau$, $q^T_\tau$, $q^T_\tau$ and, according to the above construction, $(p^T_\tau(t), q^T_\tau(t))$ and $(p^T_\tau(t), q^T_\tau(t))$, are all implicit functions of times $t_0$ and $T$. In other words, if one changes time $t_0$ or $T$, the whole construction of the set of three trajectories is different. But, if one changes $t_0$ or $T$ in an infinitesimal way, then the trajectories will only shift infinitesimally. This will simplify further calculations because of the stationarity of the action.

Remark: although $(p^T_\tau(T), q^T_\tau(T))$ is the propagation of $(p^T_\tau(t), q^T_\tau(t))$ with complex time $\Delta \tau$ and Hamiltonian $H_\tau$, $(p^T_\tau(t), q^T_\tau(t))$ is not equal to the propagation of $(p^T_\tau(t_0), q^T_\tau(t_0))$ with complex time $-\Delta \tau$ and Hamiltonian $H_{t_0}$, because (59) does not commute with (58), as explained in the paragraph before (46). If they did commute then the whole action would be the integral of an exact 1 form, so it would only depend on initial and final conditions $(p^T_\tau(t_0), q^T_\tau(t_0))$ and $(p^T_\tau(t_0), q^T_\tau(t_0))$, that is, it would be possible to deform the triple trajectory
\[
(p_{\star}^e(t_0), q_{\star}^e(t_0)) = (R_{n,T})^{-1}(p_{\star}^e(t_0), q_{\star}^e(t_0))
\]

\[
(p_{\star}^e(T), q_{\star}^e(T)) = C_{\xi, T}^{e}(p_{\star}^e, q_{\star}^e)
\]

Figure 2. The application \(M_{i_0,T} \alpha\) maps \((p_{\star}^e, q_{\star}^e)\) to \(M_{i_0,T} \alpha\)(p\(_\star\)T, q\(_\star\)T) = (p, q).

\[
(p^e_{\star}(t_0), q^e_{\star}(t_0)) = (R_{n,T})^{-1}(p^e_{\star}(t_0), q^e_{\star}(t_0))
\]

\[
(p^e(T), q^e(T)) = C_{\xi, T}^{e}(p^e_{\star}, q^e_{\star})
\]

Figure 3. Whereas \((p^e(T), q^e(T))\) is the propagation of \((p^e_{\star}(t_0), q^e_{\star}(t_0))\) with complex time \(\Delta \tau\), \((p^e_{\star}(t_0), q^e_{\star}(t_0))\) is not equal to the propagation of \((p^e(t_0), q^e(t_0))\) with complex time \(-\Delta \tau\). See the illustration on figure 3. For additional remarks on this complex structure, see appendix B.

One has finally

\[
[u(t_0, T)e^{-i\beta T} u(t_0, T)]_W(p, q) \equiv e^{\frac{i}{\hbar}[p\langle (x_{\xi, T}(t_0) - x_{\xi, T}(t_0)) + x_{\xi, T}(t_0) - x_{\xi, T}(t_0) \rangle + x_{\xi, T}(t_0) - x_{\xi, T}(t_0); x_{\xi, T}(t_0) - x_{\xi, T}(t_0), t_0; \langle (x_{\xi, T}(t_0) - x_{\xi, T}(t_0)), t_0, t_0 \rangle}].
\]

(74)

Then we define \(G^{(b)}_{T}(p, q)\) by

\[
-\Delta \tau G^{(b)}_{T}(p, q) = S_{tot}(p, q, Q^*, q^*_1, q^*_2, t_0, T).
\]

(75)

The superscript \((t_0)\) in \(G^{(b)}_{T}(p, q)\) means to distinguish the argument of the exponential in \([\hat{u}(t_0, T)e^{-i\beta T} \hat{u}(t_0, T)]_W(p, q)\) from the argument of the exponential in \(e^{-i\beta T}\)_W\((p, q)\), which would simply be \(G_T(p, q)\).
The time evolution of $G_T^{(b)}(p,q)$ can be evaluated in the same way as $G_t(p,q)$ in the previous subsection. One can indeed write

$$\frac{d}{dT}S_{\text{tot}} = \frac{\partial}{\partial T}S_{\text{tot}} + \frac{\partial}{\partial Q}S_{\text{tot}} \frac{\partial Q}{\partial T} + \frac{\partial}{\partial q_1}S_{\text{tot}} \frac{\partial q_1}{\partial T} + \frac{\partial}{\partial q_2}S_{\text{tot}} \frac{\partial q_2}{\partial T}$$

$$= \frac{\partial}{\partial T}S_{\text{tot}}$$

$$= \frac{\partial}{\partial T}S_+ + \frac{\partial}{\partial T}S_- + \frac{\partial}{\partial T}S_T. \quad (76)$$

because the $Q$, $q_1$ and $q_2$ derivatives of $S_{\text{tot}}$ are equal to 0 from stationary phase conditions (61), (62) and (63). Then, from (24), one has

$$\frac{\partial}{\partial T}S_+ (q_+(t_0), t_0; q_+(T), T) = -H_T (p_+(T), q_+(T))$$

$$\frac{\partial}{\partial T}S_- (q_-(t_0), t_0; q_-(T), T) = -H_T (p_-(T), q_-(T)) \quad (77)$$

whereas, with the same arguments of stationarity used in (49) to prove (50), one has

$$\frac{\partial}{\partial T}S_T (q_T(t_\tau), t_\tau; q_T(T), T_\tau) = - \int_{t_\tau}^{T_\tau} \partial_T H_T (p_T(\tau), q_T(\tau)) \, d\tau. \quad (78)$$

Further, the energy is conserved along the imaginary time trajectory (59), therefore $H_T (p_+(T), q_+(T)) = H_T (p_-(T), q_-(T))$, keeping in mind (65) and (66). Therefore only remains

$$\frac{d}{dT} \left( G_T^{(b)}(p,q) \right) = \frac{1}{\Delta_T} \int_{T_\tau}^{T_\tau} \partial_T H_T (p_T(\tau), q_T(\tau)) \, d\tau. \quad (79)$$

We note that it is the same expression as (50), except that the complex arc $(p_T(\tau), q_T(\tau))$ has been propagated, so $(p,q)$ is no longer the center of its chord. Let us then define $(\tilde{p}(T), \tilde{q}(T))$ as the center of the chord to the imaginary arc $\left\{ (p_T(\tau), q_T(\tau)) : \tau \in [t_\tau, T_\tau] \right\}$, that is, remembering (65) and (66),

$$\tilde{p}(T) = \frac{p_+(T_\tau) + p_+(T)}{2} = \frac{p_+(T) + p_+(T)}{2}$$

$$\tilde{q}(T) = \frac{q_+(T_\tau) + q_+(T)}{2} = \frac{q_+(T) + q_+(T)}{2}. \quad (80)$$

$(\tilde{p}(T), \tilde{q}(T))$ is then our ‘pseudo classical trajectory’, it is like the real shadow of the couple of complex Hamiltonian trajectories $(p_+, q_+)$ and $(p_-, q_-)$, as is illustrated on figure 4.

Hence, we have

$$\frac{d}{dT} \left( G_T^{(b)}(p,q) \right) = \partial_T G_T(p(T), q(T)). \quad (81)$$

Equation (81) actually looks like a backward Liouville propagation of the function defined by (50). The difference is that, in the Liouville case, $(p(T), q(T))$ is the classical propagation of $(p,q)$, whereas here, $(\tilde{p}(T), \tilde{q}(T))$ is the average of two classical propagations. We have

$$\lim_{\Delta T \to 0} (\tilde{p}(T), \tilde{q}(T)) = (p(T), q(T)). \quad (82)$$
3.3. A semiclassical Jarzynski identity

We define the semiclassical work along a trajectory \((\hat{p}(t), \hat{q}(t))\) as

\[
\mathcal{W}_{t_0, T}(p, q) = \int_{t_0}^{T} \partial_t G_t(\hat{p}(t), \hat{q}(t)) \, dt.
\] (83)

According to (81) one has

\[
\mathcal{W}_{t_0, T}(p, q) = \int_{t_0}^{T} d \left( [G_{t_0}^{(\hat{p})}(p, q)] / dt \right) dt = G_{T}^{(\hat{p})}(p, q) - G_{t_0}(p, q)
\] (84)

that is, the pseudo-work is the difference between the final and initial pseudo-energies. This allows us to follow the steps of the original Jarzynski proof in [1]. Let \(G_t(p, q)\) be the pseudo-Hamiltonian associated with \(H_t(p, q)\), and

\[
Z_{sc}(t) = \int \int e^{-\beta G_t(p, q)} \, dp dq \equiv e^{-\beta F_{sc}(t)}.
\]

The average of the exponential of the pseudo-work \(\mathcal{W}\), in the sense defined by the expression (15), is given by

\[
\left\langle e^{-\beta \mathcal{W}_{t_0, T}} \right\rangle = \int \int \rho_T(p, q) e^{-\beta \mathcal{W}_{t_0, T}} \, dp dq = \int \int \frac{e^{-\beta G_0(p, q)}}{Z_{sc}(t_0)} e^{-\beta \frac{\partial}{\partial \hat{q}} \partial_t G_t(\hat{p}(t), \hat{q}(t))} \, dp dq = \int \int \frac{e^{-\beta G_0(p, q)}}{Z_{sc}(t_0)} e^{-\beta \left( G_T^{(\hat{p})}(p, q) - G_0(p, q) \right)} \, dp dq = \int \int \frac{1}{Z_{sc}(t_0)} e^{-\beta G_T^{(\hat{p})}(p, q)} \, dp dq = \frac{Z_{sc}(T)}{Z_{sc}(t_0)} = e^{-\beta \Delta F_{sc}}.
\] (85)
with
\[ Z_{sc}(T) = \oint e^{-\beta G_{t0}(p,q)} dp dq \approx \int_{\hbar \to 0} e^{-\beta G_{t0}(p,q)} dp dq = \int_{\hbar \to 0} e^{-\beta G_{t0}(p,q)} dp dq = \int_{\hbar \to 0} e^{-\beta \hat{H}_0} e^{-\beta G_{t0}(p,q)} \hat{U}(t_0, T) \hat{U}^\dagger(t_0, T) \frac{d}{dT} \hat{G}_{t0}(\hat{p}, \hat{q}) d\hat{p} d\hat{q} = \int_{\hbar \to 0} e^{-\beta G_{t0}(p,q)} dp dq. \] (86)

Finally, we have obtained a Jarzynski identity in the semiclassical limit
\[ \int e^{-\beta G_{t0}(p,q)} dp dq = \int e^{-\beta G_{t0}(p,q)} dp dq. \]

where the pseudo-work \( W_{t0,T}(p,q) = \int_{t_0}^{T} \partial_t \hat{G}_{t}(\hat{p}, \hat{q}) dt \) is evaluated along the pseudo-trajectory \( (\hat{p}(t), \hat{q}(t)) \) which starts at \( (p, q) \), with a probability given by the thermal state \( e^{-\beta G_{t0}(p,q)} Z_{sc}(t_0) \). The average of the exponential of this pseudo-work then gives the ratio of the quantum partition functions in the semiclassical limit.

4. A solvable example: the harmonic oscillator

It is useful to illustrate formal non-equilibrium identities on some specific systems. In the case of the quantum work relations, exactly solvable models are rare and mostly limited to the harmonic oscillator, non-interacting quantum gases, or two-level systems \([65–70]\). Here, we shall apply the formulas of the previous sections to the harmonic oscillator, whose classical Hamiltonian is defined by
\[ H(p, q) = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 q^2, \] (88)
and the corresponding quantum Hamiltonian is
\[ \hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + \frac{1}{2} m \omega^2 q^2. \] (89)

4.1. Exact canonical distribution in Weyl representation

In order to calculate the canonical distribution in Weyl representation, we decompose the density operator of the thermal state in the Fock states \( |n\rangle \), and then use the Weyl representation of a projector on a Fock state, \( |n\rangle \langle n| \), which is known to be \([53, 56]\):
\[ W_n(p, q) = \frac{(-1)^n}{\pi \hbar} e^{\frac{2\pi i \hbar H(p,q)}{\hbar \omega}} L_n \left( \frac{4}{\hbar \omega} H(p, q) \right). \] (90)
Then, we have
\[ e^{-\beta \hat{H}} = \sum_n e^{-\beta \hbar \omega (n+1/2)} |n\rangle \langle n|. \] (91)

It is also useful to introduce
\[ e^{i\beta \hat{H}} = \sum_n e^{i\beta \hbar \omega (n+1/2)} |n\rangle \langle n|. \] (92)
By virtue of the linearity of the Weyl transform, the Weyl symbol of $e^{-\beta \hat{H}}$ is given by
\[
\left[ e^{-\beta \hat{H}} \right]_{W}(p, q) = \sum_{n} e^{-\beta \hbar (n+1/2)} e^{\frac{-\beta \hbar}{\pi} e^{H(p, q)} L_{n} \left( \frac{4}{\hbar \omega} H(p, q) \right)},
\]
where we recognize the generating function of the Legendre polynomials,
\[
\sum_{n} X^{n} L_{n}(Y) = \frac{e^{XY}}{1-X},
\]
from which we deduce that
\[
\left[ e^{-\beta \hat{H}} \right]_{W}(p, q) = \frac{1}{2\pi \hbar} \frac{\cosh (\beta \hbar \omega / 2)}{\sinh (\hbar \beta \omega / 2)} \exp \left[ -\frac{2}{\hbar \omega} \tanh (\frac{\beta \hbar \omega}{2}) H(p, q) \right].
\]

4.2. Canonical distribution from the stationary phase approximation

Dealing with a harmonic oscillator, we expect the stationary phase method to be exact. The imaginary time trajectory can simply be obtained. Starting from the real intersection of the complex arc with the real plane, $(p^{\star}c, q^{\star}c)$, it is given by
\[
p^{\star}(\tau) = p^{\star} \cos \omega \tau - \frac{m \omega q^{\star}}{2} \sin \omega \tau,
\]
\[
q^{\star}(\tau) = q^{\star} \cos \omega \tau + \frac{p^{\star}}{m \omega} \sin \omega \tau.
\]
Hence, from (27), where the above choice of origin implies that $\tau_{1} = -\Delta \tau / 2$ and $\tau_{1} = \Delta \tau / 2$, we obtain
\[
S = -i \left( \frac{(p^{\star}c)^{2}}{2 m} - \frac{1}{2} m \omega^{2} (q^{\star}c)^{2} \right) \frac{\sinh (\hbar \beta \omega)}{\omega} = \frac{i m \omega \cosh (\hbar \beta \omega)(q^{\star}c)^{2} + (q^{\star}c)^{2} - 2 q^{\star}q^{\star}c}{\sinh (\hbar \beta \omega)}.
\]
On the other hand, from the relation
\[
pQ^{*} = \frac{p^{\star}}{2} \left( \frac{\Delta \tau}{2} \right) + p^{\star} \left( \frac{-\Delta \tau}{2} \right) \left( q^{\star} \left( \frac{\Delta \tau}{2} \right) - q^{\star} \left( \frac{-\Delta \tau}{2} \right) \right),
\]
we deduce
\[
\frac{i}{\hbar} \left( S^{*} - pQ^{*} \right) = -\frac{1}{\hbar \omega} \sinh (\omega h \beta) \left( \frac{(p^{\star}c)^{2}}{2 m} + \frac{1}{2} m \omega^{2} (q^{\star}c)^{2} \right).
\]
Noting that
\[
p = \frac{p^{\star}}{2} \left( \frac{-\Delta \tau}{2} \right) + p^{\star} \left( \frac{\Delta \tau}{2} \right) = p^{\star} \cosh \frac{\omega h \beta}{2},
\]
\[
q = \frac{q^{\star}}{2} \left( \frac{-\Delta \tau}{2} \right) + q^{\star} \left( \frac{\Delta \tau}{2} \right) = q^{\star} \cosh \frac{\omega h \beta}{2},
\]
we conclude, from (43) and (44), that
\[ e^{-\beta G(p,q)} = \frac{1}{2\pi\hbar \cosh \left( \frac{\beta \omega}{2} \right)} \exp \left[ -\frac{2}{\hbar \omega} \tanh \left( \frac{\beta \omega}{2} \right) H(p,q) \right] \] (101)
and we recover expression (95).

4.3. Quantum power and pseudo-work

The Jarzynski power of the Hamiltonian (88) with time dependent \( \omega \) is given by
\[ \partial_t H_t = m \dot{\omega} \omega_t q^2. \] (102)
Applying equation (50), we obtain
\[ \partial_t G_t(p,q) = \frac{1}{\hbar} m \omega_t \int \frac{q^* c}{c} (q^*(\tau))^2 d\tau \]
\[ = -\frac{1}{\hbar} m \omega_t \int \frac{q^* c}{c} \left[ \left( \frac{q^* c}{c} \right)^2 \cosh(\omega_t t') - \left( \frac{p^* c}{c} \right)^2 \sinh(\omega_t t')^2 + 2i \frac{m}{\hbar \omega_t} p^* c q^* c \times \cosh(\omega_t t') \sinh(\omega_t t') \right] d\tau' \]
\[ = \frac{1}{\hbar} m \omega_t \left[ \left( \frac{q^* c}{c} \right)^2 \left( \frac{\sinh(\omega_t \beta \hbar \omega)}{2 \omega_t} + \frac{h \beta}{2} \right) - \left( \frac{p^* c}{c} \right)^2 \left( \frac{\sinh(\omega_t \beta \hbar \omega)}{2 \omega_t} - \frac{h \beta}{2} \right) \right]. \] (103)
which, using equation (100), leads to
\[ \partial_t G_t(p,q) = \frac{\dot{\omega}}{\omega_t} \frac{2}{1 + \cosh(\beta \hbar \omega)} \left[ \frac{1}{2} m \omega_t q^2 \left( \frac{\sinh(\beta \hbar \omega)}{\beta \hbar \omega} \right) + 1 \right] + \frac{p^2}{m} \left( 1 - \frac{\sinh(\beta \hbar \omega)}{\beta \hbar \omega} \right). \] (104)

One can verify that
\[ \lim_{\beta \hbar \omega \to 0} \partial_t G_t(p,q) = m \omega_t \omega_t \left( \lim_{\beta \hbar \omega \to 0} q^* c \right)^2 = m \omega_t \omega_t q^2 = \partial_t H_t(p,q) \] (105)

Remark: we note that the pseudo-trajectory \( (\hat{p}(t), \hat{q}(t)) \) actually coincides with the classical trajectory \( (p(t), q(t)) \) because of the linearity of the dynamics of the harmonic oscillator with respect to the initial conditions,
\[ \begin{pmatrix} p(t) \\ q(t) \end{pmatrix} = \begin{pmatrix} a(t) & b(t) \\ c(t) & d(t) \end{pmatrix} \begin{pmatrix} p(0) \\ q(0) \end{pmatrix}. \] (106)

5. Conclusion

We have derived a formal Jarzynski identity in the Weyl representation, whose classical limit is the celebrated nonequilibrium work identity for the corresponding classical Hamiltonian. This formal identity involves the average of the exponential of a pseudo-work \( \partial_t G_t \) along
pseudo-trajectories which start from initial phase space points distributed according to a thermal distribution. This average is shown to be equal to the ratio of the partition functions of the semiclassical thermal distribution which is approximately equal to the ratio of the quantum partition functions in the semiclassical regime—as long as the semiclassical Van Vleck propagator can be considered to be valid approximation. In other words, we have obtained a semiclassical estimate of the quantum free energy from a $\hbar$ correction of the Jarzynski identity which involve only classical quantities. This relation has been verified for the quantum harmonic oscillator.

The logical path of the present work can be summarized by the following diagram, which explains that we have combined the Weyl quantization scheme with a semiclassical (i.e. stationary phase) calculation and draws a parallel between the classical derivation of Jarzynski and its mirror image in the Weyl quantum phase space:

$$e^{-\beta H_t(p,q)} \xrightarrow{\text{Work}} W_t(p,q) = \int_0^1 \frac{\partial H_t}{\partial q'} (p(t'), q(t')) \, dt' \xrightarrow{\text{Jarzynski}} \iint \frac{e^{-\beta H_t(p,q)}}{Z_t^{(\text{class})}} e^{-\beta W_t(p,q)} \, dpdq = \frac{Z_{\text{class}}(t)}{Z_{\text{class}}(0)}$$

A natural extension of this study would be to use the formal identity in the Weyl space to calculate quantum corrections to the classical Jarzynski formula—order by order with respect to $\hbar$—and to find some geometric interpretation of these corrections. It would also be interesting to compare the pseudo-work defined here with the work operator defined for Lindblad equations [32], in the markovian framework of an open system constantly monitored by its environment.

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Appendix A. Other trajectories

The approach we followed led us to define a pseudo-Hamiltonian $\Gamma_t(p,q)$, whose semiclassical approximation is $G_t(p,q)$. It might have seemed natural to use this pseudo-Hamiltonian as a proper classical-like Hamiltonian, and generate real classical trajectories $(p_t(t), q_t(t))$ directly from Hamilton equations

$$\dot{p}_t(t) = -\frac{\partial \Gamma_t}{\partial q}(p_t(t), q_t(t))$$

$$\dot{q}_t(t) = \frac{\partial \Gamma_t}{\partial p}(p_t(t), q_t(t)).$$

(A1)
From the structure of these equations, we would then automatically have
\[
\frac{d}{dt} \Gamma_t(p_t, q_t) = \frac{\partial}{\partial t} \Gamma_t(p_t, q_t),
\]
(A2)

which is enough to derive a Jarzynski identity, by following exactly the classical proof for a Hamiltonian closed system as presented in [1]. It would give simply, by using the same argument of symplecticity of trajectories,
\[
\int \frac{e^{-\beta \Gamma_0(p_t(0), q_t(0))}}{Z(t_0)} e^{-\beta \int_0^t \partial_t \Gamma_t(p_t(t'), q_t(t')) dt'} \, dp_t(t_0) dq_t(t_0) = \frac{1}{Z(t_0)} \int e^{-\beta \Gamma_0(p_T(t), q_T(t))} \, dp_t(t_0) dq_t(t_0) = \frac{Z(T)}{Z(t_0)},
\]
(A3)

where the second line uses the fact that the Jacobian of \((p_t(0), q_t(0)) \mapsto (p_T(t), q_T(t))\) is equal to 1, because of symplecticity.

We did not retain this option because, although the proof is formally correct, we could not find any quantum signification to these trajectories in terms of the Weyl representation of a quantum evolution. On the other hand, our pseudo-trajectory \((\tilde{p}(t), \tilde{q}(t))\) naturally describes the Weyl representation of the quantum evolution of an operator, in the semiclassical limit. We have indeed,
\[
[\tilde{U}(t_0, T)\hat{A}\tilde{U}(t_0, T)]_W(p, q) = \hat{A}(\tilde{p}(T), \tilde{q}(T)).
\]
(A4)

The example of the harmonic oscillator \(H_t(p, q) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2\) is quite suggestive here. The pseudo-Hamiltonian \(\Gamma_t(p, q)\) is just the proper Hamiltonian multiplied by \(\lambda = \frac{1}{\hbar} \tanh \frac{\beta \hbar \omega}{2}\), and therefore the classical-like trajectory generated by \(\Gamma_t(p, q)\) is a classical trajectory of the Harmonic oscillator, but where the time has been scaled by \(\lambda\). This obviously comes from the Hamilton equations,
\[
\dot{p}_t(t) = -\lambda \frac{\partial H_t}{\partial q}(p_t(t), q_t(t))
\]
\[
\dot{q}_t(t) = \lambda \frac{\partial H_t}{\partial p}(p_t(t), q_t(t)),
\]
(A5)

which can be written
\[
\frac{\partial p_t}{\partial (\lambda t)} = -\frac{\partial H_t}{\partial q}(p_t(\lambda t), q_t(\lambda t))
\]
\[
\frac{\partial q_t}{\partial (\lambda t)} = \frac{\partial H_t}{\partial p}(p_t(\lambda t), q_t(\lambda t)).
\]
(A6)
On the other hand, for the Harmonic oscillator, the pseudo-trajectory \((\dot{p}(t), \dot{q}(t))\) is exactly the classical trajectory \((p(t), q(t))\) with the correct time \(t\),
\[
\dot{p}(t) = -\frac{\partial H}{\partial q}(p(t), q(t))
\]
\[
\dot{q}(t) = \frac{\partial H}{\partial p}(p(t), q(t)), \quad \text{(A7)}
\]
which suggests that this choice is indeed more natural.

### Appendix B. Complex symplectic structure

The complex structure of the trajectories is made of two types of trajectories, the imaginary ‘formal time’ trajectories \((\dot{p}^c(t), \dot{q}^c(t))\), and the real time ones, \((\dot{p}^r(t), \dot{q}^r(t))\) and \((\dot{p}^{\ast}(t), \dot{q}^{\ast}(t))\). They do not commute, therefore the mixed complex space trajectories that we consider cannot be considered as the analytical continuation of classical phase space \((p(t), q(t))\).

Obviously, freezing the time real \(t\) of the Hamiltonian \(H(p, q)\) and propagating through Hamiltonian dynamics with complex formal time, like for instance (59) if one restricts to purely imaginary formal time, will generate trajectories whose reunion is the manifold \(H(p, q) = E\), where \(E\) is a complex constant. For instance, in the scheme of figure 4, the energy \(E_c = H_0(\dot{p}^c(\tau), \dot{q}^c(\tau))\), along the arc which goes from \((\dot{p}^c(\tau_i), \dot{q}^c(\tau_i))\) to \((\dot{p}^c(\tau_t), \dot{q}^c(\tau_t))\), is a real constant, because the arc crosses the real plane \((\text{Re}(p), \text{Im}(q))\) at \((\dot{p}^c, \dot{q}^c)\), and the Hamiltonian is real.

On the other hand, the energy is not conserved any more through the real time propagations \((\dot{p}^r(t), \dot{q}^r(t))\) and \((\dot{p}^{\ast}(t), \dot{q}^{\ast}(t))\), driven by (58). Still, if we define \(E_+(t) = H_l(\dot{p}^r(t), \dot{q}^r(t))\) and \(E_-(t) = H_l(\dot{p}^{\ast}(t), \dot{q}^{\ast}(t))\), then we have \(E_+(t) = E_-(t)\), that is, both energies are complex conjugate. Also, we have \(E_+(t_0) = E_-(t_0) = E_c \in \mathbb{R}\), that is, the energy is initially real at \(t = t_0\), then they draw two complex conjugate branches until \(t = T\). The midpoint of the final tips of these two complex conjugate branches is the real phase space point \((p, q)\) where the Weyl function is evaluated (see figure 4).

Let us follow for instance \((\dot{p}^r(t), \dot{q}^r(t))\), and then let us freeze the time \(t\) at a later value \(t = t_1 > t_0\). Then, propagating from \((\dot{p}^r(t_1), \dot{q}^r(t_1))\) with complex formal time would generate a new set of trajectories whose reunion is the manifold \(\{(p, q) \in \mathbb{C}^2\text{ such that } H_l(p, q) = E_c, \quad \text{where } E_l(t_1) \in \mathbb{C}\}\), since \(H_l(p, q) = H_0(\dot{p}^c(t_1), \dot{q}^c(t_1)) = E_c\). This new manifold intersects the initial \(E_l\) manifold.

To resume, for a fixed time \(t\), the whole two dimensional complex phase space \((p, q) \in \mathbb{C}^2\) can be organized as a foliation \(\mathcal{F}\) of one complex dimension manifolds. Each one of this complex manifold is stable through the Hamiltonian dynamics generated by \(H_l\) with frozen time dependence \(t\), and it can be identified with \(\{(p, q) \in \mathbb{C}^2\text{ such that } H_l(p, q) = E\}\), with some \(E \in \mathbb{C}\), so we may call it \(\mathcal{L}_l(E)\). The reunion of all the \(\mathcal{L}_l(E)\) for all values of \(E\) gives back \(\mathbb{C}^2\). In particular, every imaginary formal time dynamics (59) lives on such a manifold \(\mathcal{L}_l(E)\). However, changing time \(t\) changes the whole foliation. As a consequence, a real time trajectory \((p(t), q(t))\), defined by (58), which crosses a leave \(\mathcal{L}_l(E)\) at time \(t\), will then cross an other leave \(\mathcal{L}_{l+\partial t}(E + dE)\) at time \(t + dt\), with \(dE\) defined by
\[
dE = \frac{d}{dt} H_l(p(t), q(t)) dt = \frac{\partial}{\partial t} H_l(p(t), q(t)) dt, \quad \text{(B1)}
\]
so \( \frac{dE}{dt} \) is a function of the trajectory \((p(t), q(t))\). Although \( \mathcal{L}_t(E + \Delta E) \) does not intersect \( \mathcal{L}_t(E) \), \( \mathcal{L}_{t+\Delta t}(E + \Delta E) \) can \textit{a priori} intersect \( \mathcal{L}_t(E) \) at points \((p_a, q_a)\) solutions of

\[
\begin{aligned}
H_t(p_a, q_a) &= E + \Delta E \\
H_t(p_a, q_a) &= E,
\end{aligned}
\]  

(B2)

that is

\[
\begin{aligned}
H_t(p_a, q_a) &= E \\
\frac{\partial}{\partial t}H_t(p_a, q_a) &= \frac{\partial}{\partial t}H_t(p(t), q(t)).
\end{aligned}
\]  

(B3)

For instance, if \( H_t(x) = H_0(x) + F_t \cdot x \), where \( x = (p, q) \), then these equations become

\[
\begin{aligned}
H_t(x_a) &= E \\
\dot{x}_a &= F_t \cdot x(t),
\end{aligned}
\]  

(B4)

which implies that \( x_a \) is at the intersection between the complex line \( x(t) + a \mathcal{J} \dot{F}_t \), \( a \in \mathbb{C} \) and the surface of constant energy \( E \). In other words, \( x_a = x(t) + a \mathcal{J} \dot{F}_t \), where \( a \in \mathbb{C} \) is such that

\[
H_t(x(t) + a \mathcal{J} \dot{F}_t) = E.
\]  

(B5)

As soon as \( H_t \) is quadratic or more, there can be other solutions than \( a = 0 \).

A natural symplectic structure can be attached to each manifold \( \mathcal{L}_t(E) \) by using Hamilton’s equation (59), generalized to arbitrary complex \( \tau \), as Schwartz identities. On the other hand, the real time dynamics, driven by (58), can be supplied with an other symplectic structure, adding \((E, t)\) as an extra couple of canonical variables to \((p, q)\), and this structure can also be extended to complex \((E, t)\). However, how to connect both symplectic structures is not clear to us by now.

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