Non-hermitian quantum thermodynamics

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Thermodynamics is the phenomenological theory of heat and work. Here we analyze to what extent quantum thermodynamic relations are immune to the underlying mathematical formulation of quantum mechanics. As a main result, we show that the Jarzynski equality holds true for all non-hermitian quantum systems with real spectrum. This equality expresses the second law of thermodynamics for isothermal processes arbitrarily far from equilibrium. In the quasistatic limit however, the second law leads to the Carnot bound which is fulfilled even if some eigenenergies are complex provided they appear in conjugate pairs. Furthermore, we propose two setups to test our predictions, namely with strongly interacting excitons and photons in a semiconductor microcavity and in the non-hermitian tight-binding model.

More and more non-hermitian systems are becoming experimentally accessible1. Therefore, it has become evident that questions concerning foundations of quantum mechanics are no longer only of academic interest. Recent experiments have demonstrated that hermiticity may not be as fundamental as mandated by quantum mechanics4,5. For instance, in spontaneous PT-symmetry breaking has been observed indicating a condition weaker than hermiticity (namely PT3) being realized in nature. Furthermore, in6 exceptional eigenenergies of complex quantum mechanical theory has to be built on hermitian operators is rather mathematically convenient than being of mathematical necessity needed for a proper probabilistic, physical theory. To demand, however, that any quantum system evolving under unitary dynamics the so-called two-time energy measurement approach has proven to be practical and powerful. In this paradigm, quantum work is determined by projective energy measurements at the beginning and the end of a process induced by an externally controlled Hamiltonian. The predictions, namely with strongly interacting excitons and photons in a semiconductor microcavity and in the non-hermitian tight-binding model.

Very recently, it has become evident that for a special class of non-hermitian systems, namely in PT-symmetric quantum mechanics6,7, the quantum Jarzynski equality holds without modification8. For isolated quantum systems evolving under unitary dynamics the so-called two-time energy measurement approach has proven to be practical and powerful. In this paradigm, quantum work is determined by projective energy measurements at the beginning and the end of a process induced by an externally controlled Hamiltonian. The Jarzynski equality9 together with subsequent Nonequilibrium Work Theorems, such as the Crooks fluctuation theorem10, is undoubtedly among the most important breakthroughs in modern Statistical Physics11. Jarzynski showed that for isothermal processes the second law of thermodynamics can be formulated as an equality, no matter how far from equilibrium the system is driven12, \( \langle \exp(-\beta W) \rangle = \exp(-\beta \Delta F) \). Here \( \beta \) is the inverse temperature of the environment, and \( \Delta F \) is the free energy difference, i.e., the work performed during an infinitely

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A non-hermitian Hamiltonian such as (1) is called pseudo-hermitian if a proper metric operator exists such that $H_{\alpha\beta} = g_{\alpha\beta} E_{\alpha}$. In general, the energy eigenvalues are complex, and the eigenvalue problem reads

$$H\psi_{\alpha} = E_\alpha \psi_{\alpha}, \quad H^\dagger \phi_{\alpha} = E_\alpha \phi_{\alpha},$$

with $\langle \psi_{\alpha} | \phi_{\beta} \rangle = \delta_{\alpha\beta} \delta_{\tau_0}$ and $\sum_{\alpha} \langle \psi_{\alpha} | \phi_{\alpha} \rangle = 1$. A non-hermitian Hamiltonian such as (1) is called pseudo-hermitian if $g$ exists such that

$$H^\dagger = gH g^{-1} \quad \text{and} \quad g = g^\dagger.$$

It does exist if and only if either all eigenenergies are real or complex ones appear in conjugate pairs with the same degeneracy. If none of those criteria are met $H$ is generally non-hermitian; yet it still can be useful, e.g. for an effective description of open quantum systems. However, when heat is exchanged the two-time energy measurement can no longer describe the work done during a thermodynamic process. Therefore we shall not focus on such cases here. Another interesting class relates to systems that interact with environments, but do not exchange heat. This phenomenon is called dephasing (loss of information). For such systems, work can still be determined by the two-time energy measurement and the Jarzynski equality holds as well.

Condition (2) assures that $H$ is, in fact, hermitian however with respect to a new inner product, namely

$$\langle \psi | \phi \rangle_g := \langle \psi | g \phi \rangle.$$

Note that $g$ always exists such that $\langle \psi | \phi \rangle_g$ is positive-definite (this is a genuine inner product), and it can be found if and only if the spectrum of $H$ is real. To make a consistent definition of work for a quantum system within the two-time energy measurement paradigm its spectrum has to be real. Therefore, unless stated otherwise, we shall always assume this to be the case. Then, Eq. (2) can be fulfilled by the following positive-definite operators ($g$ is a proper metric operator)

$$g = \sum_{\alpha} | \phi_{\alpha} \rangle \langle \phi_{\alpha} |, \quad g^{-1} = \sum_{\alpha} | \psi_{\alpha} \rangle \langle \psi_{\alpha} |.$$

Often, $g$ fulfilling (2) can be deduced easily from physical properties such as the parity reflection or time reversal. Nevertheless, only Eq. (4) assures that $\langle \psi | \psi \rangle_g > 0$ for all states $\psi = 0$. This means that the proper metric may reflect ‘symmetries’ that are hidden from the observer. For instance, if a rotation $V$ exists such that $V^\dagger HV$ is diagonal in an orthonormal basis, then $g = V^\dagger V$. This follows directly from Eq. (4). The last formula is especially useful in practice. It allows one to find the metric by analyzing an experimental setup (e.g. inspecting the orientation of the axis, etc.).

In the following we only consider cases where changes of the Hamiltonian are induced by a time-dependent thermodynamic process $\lambda_t$, that is to say $H_t = H(\lambda_t)$. If such changes occur then the metric operator satisfying Eq. (2) is time-dependent. Nevertheless, the dynamics is still governed by a time-dependent Schrödinger equation. However, a slight modification becomes necessary to preserve unitarity. The derivative with respect to time $t$. The Schrödinger equation (5) can also be rewritten in the standard form, that is, with $H_t$ being the generator. Indeed, it is sufficient to replace $\partial_t$ with a covariant derivative $D_t := \partial_t + g_t^{-1} \partial_t g_t$. By construction the unique solution to Eq. (5) obeys the relation

$$U_t g_t = g_0 U_0^{-1}, \quad \text{where} \quad g_0 := g_{t=0}.$$
This relation can be viewed as the corresponding unitarity condition similar to the "standard" one, i.e., $U_t = U_t^{-1}$.

For pseudo-hermitian systems an average value of a non-hermitian observable $A$, $\text{tr}[A]$, can be computed as

$$\text{tr}[A] = \sum_{k,\gamma} \langle \psi_{k,\gamma} | gA | \psi_{k,\gamma} \rangle.$$  

(7)

Formally, this suggests one to use the following Dirac correspondence between bra and ket vectors $|\psi\rangle \rightarrow \langle \psi|^{16}$.

**Pseudo-hermitian Jarzynski equality.** Having analyzed the mathematical structure of pseudo-hermitian quantum systems, we turn to the physical description to analyze the Jarzynski equality. Without loss of generality and to simplify our notation we assume the spectrum to be non-degenerate.

For an isolated quantum system, the work done during a thermodynamic process $\lambda$, of duration $\tau$ is commonly determined by a two-time energy measurement$^{29}$. At $t = 0$ a projective energy measurement is performed. Next, the system evolves unitarily under the generalized time-dependent Schrödinger equation (5) only to be measured again at $t = \tau$. By averaging over an ensemble of realizations of such processes one can reconstruct the distribution of work values$^{30,31}$,

$$\mathcal{P}(w) = \sum_{n,m} \delta(w - w_{nm})p_{nm}.$$  

(8)

Above, $p_{nm}$ denotes a probability that a specific transition $|\psi_{m}(\lambda_0)\rangle \rightarrow |\psi_{n}(\lambda_0)\rangle$ will occur, whereas $w_{nm} = E_{n} - E_{m}$ is the corresponding work done during this transition. It is important to stress that this work is associated with $H_{t}$ rather than $H_{t} + G$, as $G_{t}$ is a gauge field, and hence it can have no influence on physical observables$^{32}$.

The transition probability $p_{nm}$ can be seen as the joint probability that the first measurement will yield the energy value $E_{m}$ given the system has been initially prepared in a state $\rho_{\nu}$ and the probability that the outcome of the second measurement will be $E_{n}^\tau$ given the initial state $\psi_{\nu}$. Therefore,

$$p_{nm} = \text{tr}[\Pi_{\nu}\rho_{\nu}] \times \langle \psi_{m}^\tau | g^{\tau} U_{r} \psi_{n} \rangle \rangle,$$  

(9)

where $U_{r}$ denotes the evolution operator generated by $H_{t} + G_{t}$ at time $t = \tau$, whereas $\Pi_{\nu} = \langle \psi_{m}^\tau | g^{\tau} \cdot \rangle \psi_{n}$ is the projector into the space spanned by the $m$th eigenstate. Since $\Pi_{\nu}$ is not hermitian the formula for probabilities $p_{nm}$ accounts for the metric $g$ and hence differs from the one usually adopted for hermitian systems$^{31}$.

Assume the system is initially in a Gibbs state, that is $\rho_{\nu} = \exp(-\beta H_{0})/Z_{0}$ with $Z_{0} = \text{tr}[\exp(-\beta H_{0})]$ being the partition function, then

$$p_{nm} = \frac{e^{-\beta E_{m}}}{Z_{0}} \langle U_{r} g^{\tau} \psi_{m}^{\tau} | \Pi_{\nu} U_{r}^{-1} \psi_{n}^{\tau} \rangle.$$  

(10)

To obtain the last expression for $p_{nm}$ we have also invoked the unitarity condition (6). Now, the average exponentiated work can be expressed as

$$\langle e^{-\beta W} \rangle = \int dw \mathcal{P}(w) \exp(-\beta w) = \frac{1}{Z_{0}} \sum_{m,n} e^{-\beta E_{m}} \langle g^{\tau} \psi_{m}^{\tau} | U_{r} \Pi_{\nu} U_{r}^{-1} \psi_{n}^{\tau} \rangle.$$  

(11)

Finally, summing out all projectors $\Pi_{\nu}$ and taking into account that $\langle g^{\tau} \psi_{m}^{\tau} | \psi_{n}^{\tau} \rangle = 1$ we arrive at

$$\langle e^{-\beta W} \rangle = \frac{1}{Z_{0}} \sum_{m} e^{-\beta E_{m}} = \frac{Z_{\tau}}{Z_{0}} = e^{-\beta F},$$  

(12)

where $F = (-1/\beta) \ln(Z)$ is the system's free energy.

The last equation shows that the Jarzynski equality holds also for non-hermitian systems that admit real spectrum. This is our first main result. Jarzynski has shown that the second law of thermodynamics for isothermal processes can be expressed as an equality arbitrarily far from equilibrium. Our analysis has shown that this result is true for all non-hermitian systems with real spectrum.

**Carnot bound.** In the preceding section we argued that if the two-time energy measurement can be performed on a non-hermitian quantum system, then the Jarzynski equality holds as long as the eigenenergies are real. Now, we will prove that the Carnot statement of the second law is also true for all pseudo-hermitian systems.

Consider a generic system that operates between two heat reservoirs with hot, $T_{h}$, and cold, $T_{c}$, temperatures, respectively. Then, the Carnot engine consists of two isothermal processes during which the system absorbs or exhausts heat and two thermodynamically adiabatic, that is, isentropic strokes while the extensive control parameter $\lambda$ is varied$^{33,34}$. It is well established that the maximum efficiency $\eta$ for classical systems, attained in the quasi-static limit, is given by the Carnot bound$^{35-37}$:

$$\eta = 1 - \frac{T_{c}}{T_{h}} < 1.$$  

(13)

Recent years have witnessed an abundance of research$^{38-40}$ investigating whether quantum correlations can be harnessed to break this limit. Recently, the Carnot limit has been proven to be universal within the usual
framework. This limit can be seen as yet another formulation of the second law of thermodynamics for quasistatic processes. We will show that it holds for all pseudo-hermitian systems whether their spectrum is real or not.

We begin by proving that both the energy \( E = \text{tr} \{ \rho H \} \) and entropy \( S \) are real in our present framework. Indeed, from (2) it immediately follows that

\[
E^* = \text{tr} \{ g g^{-1} g H g^{-1} \} = E,
\]

with \( \rho \) being a Gibbs thermal state. Interestingly, this result holds true even if some of the eigenvalues \( E_n \) are complex. Note, in that case \( g \) exists but is not positive definite and thus cannot be expressed like in Eq. (4).

To understand why Eq. (14) holds when complex eigenvalues appear in conjugate pairs note that \( |\psi_{n,\alpha}\rangle = g^{-1} |\phi_{n,\alpha}\rangle \), and consider

\[
H |\psi_{n,\alpha}\rangle = g^{-1} H |\phi_{n,\alpha}\rangle = E_n^* |\psi_{n,\alpha}\rangle,
\]

showing that if \( E_n \) is in the spectrum of \( H \) so is \( E_n^* \). Moreover \( g^{-1} \) maps the subspace spanned by all eigenvectors belonging to \( E_n \) to that belonging to \( E_n^* \). Since \( g^{-1} \) is invertible, the mapping is one-to-one, and the multiplicity of both \( E_n \) and \( E_n^* \) is the same. An interesting realization of such systems is the non-hermitian tight-binding model.

The result (14) can also be obtained directly, that is, without invoking the metric \( g \) explicitly. Indeed, we have

\[
E = \text{tr} \{ \rho H \} = \frac{1}{Z} \sum_n E_n e^{-\beta E_n} = -\frac{1}{2Z} \frac{\partial}{\partial \beta} \sum_{n=2} \left( e^{-\beta E_n} + e^{-\beta E_n^*} \right) = E^*.
\]

In the present case, the thermodynamic entropy is given by the von Neumann entropy. The latter can be shown to be real if and only if the eigenvalues \( E_n \) are real. The result (14) can also be obtained directly, that is, without invoking the metric \( g \) explicitly. Indeed, we have

\[
dE = \text{tr} \{ \delta \rho H \} + \text{tr} \{ \rho \delta H \}.
\]

In the quasistatic regime, the second law of thermodynamics for isothermal processes states that \( dS = \beta dQ \). Combining the latter with (17) proves that (i) \( dQ \) and thus \( dE \) are real and (ii) the intuitive definitions of heat and work introduced in Ref. [44] apply also to pseudo-hermitian systems.

After completing a cycle, a quantum pseudo-hermitian heat engine has performed work \( \langle W \rangle = \langle Q_h \rangle - \langle Q_c \rangle \) and exhausted a portion of heat \( \langle Q_c \rangle \) to the cold reservoir. Therefore, the efficiency of such a device is given by

\[
\eta = \frac{\langle W \rangle}{\langle Q_c \rangle} = 1 - \frac{T_c}{T_h}.
\]

In conclusion, we have shown that the Carnot bound, which expresses the second law of thermodynamics for quasistatic processes, holds for all pseudo-hermitian systems. In contrast, the second law for arbitrarily fast processes encoded in the Jarzynski equality (12), only holds for all non-hermitian systems with real spectrum.

**Discussion**

**Example 1a.** We begin with a model for localization effects in solid state physics. The general form of its Hamiltonian in one dimension reads

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

where \( V(x) \) is a confining potential, and \( p \) and \( x \) are the momentum and position operators respectively. They obey the canonical commutation relation \([x, p] = i\hbar\). Real parameter \( \xi \) expresses an external magnetic field and \( m \) is the mass. Using the Baker-Campbell-Hausdorff formula one can verify that

\[
e^{i\xi \hat{p}} e^{-i\xi \hat{p}} = p + 2\xi [x, p] + 2\xi^2 [x, [x, p]] + \ldots = p + 2i\xi.
\]

Therefore, since \([V(x), e^{i\xi \hat{p}}] = 0\), we conclude that \( H \) is pseudo-hermitian. The metric \( g = e^{i\xi \hat{p}} \) is positive definite and thus the spectrum of (19) is real. Further, we assume that the corresponding classical potential \( V_c(x) \) has a non-vanishing second derivative, and a minimum at \( x = 0 \) (e.g. \( V_c''(0) = 0 \)). Then

\[
V_c(x) = V_c'(0)x + \frac{1}{2} V_c''(0)x^2 + O(\delta x^3) \approx \frac{1}{2} m\omega^2 x^2,
\]

where \( V_c'(0) = \frac{1}{2} m\omega^2 \) has been introduced. After quantization, the eigenvalues and eigenvectors of this non-hermitian harmonic oscillator read (for the sake of simplicity we set \( m = \hbar = 1 \) throughout)
Figure 1. Left panel: Average exponentiated work $\langle e^{-\beta W}\rangle$ (blue curve) as a function of the number of terms $N_{\text{max}}$ included in the summation (11) for the protocol (23). The function quickly converges to $e^{-\beta \Delta F}$ (red curve) showing that the Jarzynski equality (12) holds. Right panel: $\langle W_{\text{irr}}\rangle = \langle W \rangle - \Delta F$ as a function of $\tau$ which relates to the speed at which the energy is supplied to the system. The irreversible work $\langle W_{\text{irr}}\rangle \to 0$ as $\tau$ approaches the quasistatic regime. The inset (red curve) shows the irreversible work calculated for a linear protocol, $\omega(t) = \omega_1 + (\omega_f - \omega_1)t/\tau$. We see that it takes longer for the system to reach its quasistatic regime. Parameters used in the numerical simulations are: $\omega_f = 0.2, \omega_f = 0.6, N\tau = 1.5$ (left panel) and $N\tau = 3$ (right panel); the remaining parameters were set to 1.

$\psi_n(x) := \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-x^2/2} H_n(\sqrt{\omega} x) e^{-x^2/2}$, 
$E_n = \omega \left(n + \frac{1}{2}\right)$,  
\begin{equation}
\psi_n(x) := \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-x^2/2} H_n(\sqrt{\omega} x) e^{-x^2/2}, \quad E_n = \omega \left(n + \frac{1}{2}\right),
\end{equation}
where $H_n(x)$ are the Hermite polynomials.

Now we assume that the size of this harmonic trap (e.g. $\omega$) is changed, and thus $g$ does not depend on time. Experimentally, harmonic traps are sensitive to initial excitations resulting for a discontinuity of the protocol itself at the beginning\(^45\). The most common way to minimize this effect, while quenching between $\omega_1$ and $\omega_f$ is to use functions smooth enough at the “edges”, for instance, 
\begin{equation}
\omega(t) = \frac{\omega_1 + \omega_f}{2} + \frac{\omega_1 - \omega_f}{2} \text{erf}(t/\tau), \quad -N\tau < t < N\tau
\end{equation}
where $\text{erf}(\cdot)$ denotes the error function, $\tau$ is a time scale, and $N$ is an integer emulating infinity. The transition probabilities (9) can be expressed via the following integral
\begin{equation}
P_{nm} = \frac{\exp(-\beta \omega(n + 1/2))}{\sinh(\beta \omega/2)} \int_{-\infty}^{\infty} e^{2ix} \psi_m^\tau(x) \psi_n(x, N\tau) dx,
\end{equation}
where the partition function $Z_\omega = 1/\sinh(\beta \omega/2)$ has been calculated exactly; and $\psi_n(x, N\tau) = U_{N\tau} \psi_n(x)$ is the solution of Eq. (5), with the initial condition given by (22), at $t = N\tau$. Although $\psi_n(x, N\tau)$ cannot be obtained analytically, a closed form expressed in terms of a solution to the corresponding classical equation of motion can be found (see e.g. Ref. 46).

Figure 1 (Left panel) shows the average exponentiated work $\langle e^{-\beta W}\rangle$ (blue curve) as a function of the number of terms $N_{\text{max}}$ included in the summation (11). This function quickly converges to $e^{-\beta \Delta F}$ proving that the Jarzynski equality (12) holds. On the right panel we have depicted the irreversible work $\langle W_{\text{irr}}\rangle = \langle W \rangle - \Delta F$ (blue curve) as a function of $\tau$ which determines the speed at which the energy is supplied to the system. When $\tau \to \infty$ the system enters its quasistatic regime and the irreversible work becomes negligible, that is $\langle W_{\text{irr}}\rangle \to 0^{+47,48}$. The inset (red curve) shows the irreversible work calculated for a linear protocol, $\omega(t) = \omega_1 + (\omega_f - \omega_1)t/\tau$. As we can see, it takes longer for the system to reach its quasistatic regime. Moreover, the oscillatory behavior is a signature of the initial excitation which dominates for fast quenches (small $\tau$).

**Example 1b.** Another class of systems that is used to explain localization effects relates to non-hermitian tight-binding models\(^{49,50}\). For example
\begin{equation}
H = -\frac{t}{2} \sum_{x} \sum_{i=1}^{d} \epsilon_i a_i^\dagger x a_x + \epsilon_x a_i^\dagger x a_x + \sum_{x} V_x a_i^\dagger x a_x,
\end{equation}
where $a_i^\dagger$ and $a_i$ are bosonic creation and annihilation operators respectively, $\epsilon_i$ are the unit lattice vectors, and $t$ is the hopping parameter, and $V_x$ denotes the on-site potential. Interestingly, the complex eigenvectors appear in conjugate pairs (see Eq. (2) in Ref. 41 and the discussion that follows). Therefore, this model provides another example for a building block of a non-hermitian Carnot engine.

**Example 2.** The remainder of the present work is dedicated to a careful study of a second, experimentally relevant example\(^6\). Consider a two level system described by the Hamiltonian
\begin{equation}
H = \epsilon_1 a_1^\dagger a_1 + \epsilon_2 a_2^\dagger a_2 + (\omega_1 + \omega_2)t/\tau.
\end{equation}
A simple calculation shows that

\[ H = \lambda_i \sigma_x + \lambda^* \sigma_x \sigma_z + \gamma \sigma_+ + \gamma^* \sigma_- , \]

where \( \lambda_i \) is a complex control parameter, and \( \gamma \) is a complex constant, whereas \( \sigma_x \) and \( \sigma_\pm \) are the raising and lowering fermionic operators. This simple model (26) has been extensively studied in the literature\cite{11,51,52}, and it has been also realized experimentally both in optics\cite{4} and semiconductor microcavities\cite{6}.

To make the spectrum of (26) real we set \( \lambda_i = \lambda + (\lambda_i - \lambda) t / \tau \). The linearity does not pose any restriction on our analysis as the Jarzynski equality holds for any protocol that satisfies the basic requirements imposed on them by the axiom of quantum mechanics - hermiticity. We have shown that the second law still holds for all pseudo-hermitian systems.

To investigate the dynamics of (26) we assume that \( \lambda_i \) changes on a time scale \( \tau \) in a linear manner, that is \( \lambda_i = \lambda + (\lambda - \lambda) t / \tau \). The linearity does not pose any restriction on our analysis as the Jarzynski equality holds for any protocol that satisfies the basic requirements imposed on them by the axiom of quantum mechanics - hermiticity. We have shown that the second law still holds for all pseudo-hermitian systems.

**Conclusions**

In summary, we have carefully studied thermodynamic properties of quantum systems that do not satisfy one of the basic requirements imposed on them by the axiom of quantum mechanics - hermiticity. We have shown that if quantum work can be determined by the two-time projective energy measurements, then the Jarzynski equality still holds for non-hermitian systems with real spectrum. Note, this equality expresses the second law of thermodynamics for isothermal processes arbitrarily far from equilibrium.
We have also argued that the Carnot bound is attained for all pseudo-hermitian systems in the quasistatic limit. Furthermore, we have also proposed an experimental setup to test our predictions. As elaborated in the previous section, the system in question consists of strongly interacting excitons and photons in a semiconductor microcavity. Moreover, we have investigated two non-hermitian models that were originally introduced to explain localization effects in solid state physics. The first one, a non-hermitian harmonic oscillator, was used to demonstrate the Jarzynski equality. The second one, the so-called non-hermitian tight-binding model was given as an example of a quantum system having complex eigenenergies that appear in conjugate pairs. This model provides another example of a building block of a non-hermitian Carnot engine.

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Author Contributions
B.G., S.D. and A.S. developed ideas and derived the main results. B.G. prepared Figures 1 and 2. B.G., S.D. and A.S. wrote and reviewed the manuscript.

Additional Information
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