Quantum Work and Heat

Quantum Foundations · Module 9 — Quantum Thermodynamics

Node 9.2

Position in Knowledge Graph

System: Quantum Foundations **Structural Domain:** Quantum Thermodynamics **Node:** 9.2

The first law of thermodynamics splits energy change into work and heat. In quantum mechanics this split is non-trivial: there is no self-adjoint operator whose expectation value gives "work done," and the very definition depends on how the system is probed. The **two-point measurement (TPM) scheme** is the standard operational resolution. It makes work a *stochastic variable* on a probability space defined by two projective energy measurements, and it connects directly to the fluctuation theorems of 9.3 and the engine cycles of 9.5.

Formal Definition

Let a system have a time-dependent Hamiltonian $H(t)$ over $t \in [0, \tau]$, with instantaneous spectral decomposition

$$H(t) = \sum_n E_n(t)\, \Pi_n(t).$$

The **two-point measurement protocol** is:

1. Prepare the system in the initial thermal state $\rho_0 = e^{-\beta H(0)}/Z_0$.
2. Measure $H(0)$ projectively. Outcome $E_n(0)$ occurs with probability $p_n^0 = e^{-\beta E_n(0)}/Z_0$.
3. Evolve the post-measurement state under the unitary $U_\tau = \mathcal{T} \exp\bigl(-i \int_0^\tau H(t)\, dt\bigr)$ generated by the driving protocol.
4. Measure $H(\tau)$ projectively. Outcome $E_m(\tau)$ occurs with conditional probability $p_{m|n} = |\langle m_\tau | U_\tau | n_0 \rangle|^2$.

The **work** done by the protocol in a single run is the random variable

$$W = E_m(\tau) - E_n(0),$$

with joint probability

$$P(n, m) = p_n^0\, p_{m|n}, \qquad P(W) = \sum_{n,m} P(n, m)\, \delta\bigl(W - [E_m(\tau) - E_n(0)]\bigr).$$

For an **isolated** driven system (no bath contact during $[0, \tau]$), all energy change is work and there is no heat:

$$\langle W \rangle = \mathrm{tr}(\rho_\tau H(\tau)) - \mathrm{tr}(\rho_0 H(0)).$$

For a system in contact with a bath, heat is identified through the bath's energy change:

$$Q = -\Delta E_{\text{bath}}, \qquad \Delta E_{\text{sys}} = W + Q.$$

This is the **quantum first law** at the level of averages, and at the level of individual trajectories if one also measures the bath.

Intuition

Classically, work is "the integral of force along a path" and heat is "energy flowing across a contact." Quantum mechanically this picture breaks because:

- There is no phase-space trajectory to integrate along.
- Energy is in general not even well-defined until it is measured (if $[\rho, H] \neq 0$).
- Any attempt to continuously monitor energy changes during the protocol disturbs the state and changes the dynamics.

The TPM scheme sidesteps these problems by only asking about energy at the *endpoints*. Between the two measurements the system evolves unitarily (or via a Lindblad map if the bath is present), and the "work" is whatever the energy meter says changed. The *protocol* — the time-dependent parameters of $H(t)$ — is the analogue of classical "pushing a piston." The unitary does not commute with the projectors in general, so work is genuinely stochastic: the same protocol produces a distribution $P(W)$, not a single number.

Heat, in the same scheme, is what the *bath* recorded. If you can monitor bath energy (idealized), Q is also a two-point measurement on H_{bath}. In practice you usually infer Q from an ensemble average and the first law.

Structural Role

9.2 is the bridge between equilibrium and non-equilibrium quantum thermodynamics. It takes the Gibbs state of 9.1 as the initial condition and asks: what happens when you drive the Hamiltonian away from equilibrium?

- **9.3 Fluctuation theorems** are identities on the work distribution $P(W)$. Jarzynski's equality $\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$ is a statement about the TPM distribution and requires exactly this definition of work.
- **9.5 Quantum heat engines** are cyclic protocols whose net work output is computed by averaging W over many TPM runs.
- **9.4 Landauer's principle** is the special case where the protocol erases a bit and the minimum average heat dissipated is $k_B T \log 2$.
- **9.6 Resource theories** take Gibbs-preserving or thermal operations as free and quantify work as the cost to move between non-equilibrium states.

Without the TPM scheme, none of these downstream nodes has a well-posed starting point.

Mathematical Development

Characteristic function of work

The characteristic function $\chi(u) = \langle e^{iuW} \rangle$ admits a compact two-time-correlation form:

$$\chi(u) = \operatorname{tr}\Big[e^{iuH(\tau)}\, U_\tau\, e^{-iuH(0)}\, \rho_0\, U_\tau^\dagger\Big].$$

Fourier-inverting gives $P(W)$. This representation makes the fluctuation theorems of 9.3 easy to derive: they become symmetry statements about $\chi(u)$ under $u \to -u + i\beta$.

Average work from unitary dynamics

For an isolated protocol,

$$\langle W\rangle = \sum_{n,m} p_n^0 \,|\langle m_\tau|U_\tau|n_0\rangle|^2 \,(E_m(\tau)-E_n(0)) = \mathrm{tr}(\rho_\tau H(\tau)) - \mathrm{tr}(\rho_0 H(0)),$$

so $\langle W\rangle$ coincides with the *unmeasured* expected energy change. Individual runs deviate from this average, which is why work fluctuations are non-trivial even in pure unitary evolution.

Quantum Jarzynski identity (preview of 9.3)

Direct calculation of $\langle e^{-\beta W}\rangle$ using $p_n^0 = e^{-\beta E_n(0)}/Z_0$:

$$\langle e^{-\beta W}\rangle = \sum_{n,m} \frac{e^{-\beta E_n(0)}}{Z_0}\, p_{m|n}\, e^{-\beta(E_m(\tau)-E_n(0))} = \frac{1}{Z_0}\sum_m e^{-\beta E_m(\tau)} = \frac{Z_\tau}{Z_0} = e^{-\beta \Delta F}.$$

This is the Jarzynski equality, obtained as a three-line consequence of the TPM definition.

First law for Lindblad dynamics

For an open system evolving under a time-dependent Lindblad generator $\mathcal{L}_t$, differentiate the expected energy:

$$\frac{d}{dt}\mathrm{tr}(\rho_t H(t)) = \underbrace{\mathrm{tr}(\rho_t\,\partial_t H(t))}_{\dot W} + \underbrace{\mathrm{tr}((\mathcal{L}_t\rho_t)H(t))}_{\dot Q}.$$

Work is associated with the explicit time dependence of H; heat is associated with the dissipator. Integrating gives the average first law. The TPM scheme reproduces this at the level of averages while also giving access to the *distribution* of W over trajectories.

Worked Example

Driven qubit under a sudden quench

Take $H(t) = \frac{\omega}{2}Z$ for $t<0$, then suddenly quench to $H = \frac{\omega}{2}(\cos\theta\, Z + \sin\theta\, X)$ at $t=0$, and read out the new energy immediately. Initial state is $\rho_0 = e^{-\beta H(0)}/Z_0$.

Step 1: Initial measurement. The system is diagonal in the original Z basis, so the first measurement leaves it in $|0\rangle$ or $|1\rangle$ with probabilities

$$p_0^0 = \frac{1}{1+e^{-\beta\omega}}, \qquad p_1^0 = \frac{e^{-\beta\omega}}{1+e^{-\beta\omega}}.$$

(Energies $-\omega/2$ and $+\omega/2$.)

Step 2: Unitary. The quench is instantaneous, so $U_\tau = I$ and the post-measurement state is just $|0\rangle$ or $|1\rangle$.

Step 3: Final measurement. The new Hamiltonian has eigenstates $|+_\theta\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)|1\rangle$ and $|-_\theta\rangle = -\sin(\theta/2)|0\rangle + \cos(\theta/2)|1\rangle$ with energies $\pm\omega/2$.

Overlap probabilities from $|n\rangle$ to $|\pm_\theta\rangle$:

$$p_{\pm|0} = \cos^2(\theta/2),\ \sin^2(\theta/2); \qquad p_{\pm|1} = \sin^2(\theta/2),\ \cos^2(\theta/2).$$

Step 4: Work distribution. Four outcomes with values $W \in \{0, +\omega, -\omega\}$:

- $W = 0$: start $|0\rangle$ end $|+_\theta\rangle$, or start $|1\rangle$ end $|-_\theta\rangle$.
- $W = +\omega$: start $|0\rangle$ end $|-_\theta\rangle$ (energy $-\omega/2 \to +\omega/2$).
- $W = -\omega$: start $|1\rangle$ end $|+_\theta\rangle$.

Assembling:

$$P(W = +\omega) = p_0^0 \sin^2(\theta/2), \quad P(W = -\omega) = p_1^0 \sin^2(\theta/2), \quad P(W = 0) = \cos^2(\theta/2).$$

Check Jarzynski. Compute $\langle e^{-\beta W} \rangle$:

$$\cos^2(\theta/2) + p_0^0 \sin^2(\theta/2) e^{-\beta\omega} + p_1^0 \sin^2(\theta/2) e^{+\beta\omega}.$$

Substituting $p_0^0 = 1/(1 + e^{-\beta\omega})$ and simplifying yields Z_τ/Z_0, consistent with the general identity. At $\theta = 0$ (no quench) $P(W = 0) = 1$ and all identities reduce trivially. At $\theta = \pi$ (complete flip) the distribution is maximally broad at fixed β.

Cross-Links

- **9.1 Gibbs state** — defines the initial condition for TPM protocols.
- **9.3 Fluctuation theorems** — identities on $P(W)$; Jarzynski, Crooks, Tasaki–Crooks.
- **9.5 Quantum heat engines** — work output is the TPM expectation over a cycle.
- **8.2 Lindblad equation** — separates work (from $\partial_t H$) from heat (from dissipator) at the level of averages.
- **3.x Projective measurement** — TPM is two projective measurements of $H(0)$ and $H(\tau)$.
- **Statistics** — W is a genuine random variable; $P(W)$ is a probability distribution with finite moments.

Structural Compression

Invariant: Quantum work is a stochastic variable defined by two projective energy measurements at the endpoints of a driving protocol.

Mechanism: Two-point measurement scheme. $W = E_m(\tau) - E_n(0)$ with joint probability $p_n^0 p_{m|n}$.

Cross-System Echo: Classical work is a path integral of force. Quantum work is a difference of two measurement outcomes. The first law $\Delta E = W + Q$ survives, but W and Q lose their operator identity and become distributions.

Exercises

1. Derive the characteristic function $\chi(u) = \mathrm{tr}[e^{iuH(\tau)} U_\tau e^{-iuH(0)} \rho_0 U_\tau^\dagger]$ from the TPM joint probability, and verify that $\langle W \rangle = -i\partial_u \chi|_{u=0}$ recovers the expected first-law expression.

2. Compute the full work distribution $P(W)$ for a qubit with $H(0) = \frac{\omega}{2} Z$ quenched suddenly to $H(\tau) = \frac{\omega'}{2} Z$ (pure frequency change, no rotation). Show that $P(W)$ is supported on four points and that $\langle W \rangle = (\omega' - \omega)\langle Z \rangle/2$.

3. Show that if $[H(0), H(\tau)] = 0$, the TPM work distribution coincides with the classical distribution over energy-eigenstate transitions, and $P(W)$ has no quantum-coherence contributions.

4. For a harmonic oscillator with $H(t) = \hbar\omega(t)(a^\dagger a + 1/2)$ under an adiabatic frequency ramp, show that the work distribution factors into contributions from each occupation number and that $\langle W \rangle = \hbar\Delta\omega\langle n \rangle$.
5. Derive the quantum Jarzynski identity $\langle e^{-\beta W} \rangle = e^{-\beta\Delta F}$ from the TPM definition in under five lines, and identify exactly where the assumption "initial state is Gibbs" enters.
6. Consider an open-system protocol where H is held fixed but the system is put in contact with a bath. Show that the TPM scheme assigns $W = 0$ on every run, while the average energy change equals the heat absorbed from the bath.
7. **Argue, structurally**, why there cannot exist a self-adjoint "work operator" $\hat{W}$ whose expectation value $\langle \hat{W} \rangle$ in the initial state agrees with the TPM average $\langle W \rangle$ *and* whose variance agrees with the TPM variance, for all protocols. Use the fact that variances of self-adjoint operators are basis-independent but TPM variances depend on the initial-energy eigenbasis.

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Concepts: expectation-value, unitary-evolution, random-variables
Prerequisites: 9.1
Enables: 9.3, 9.5

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