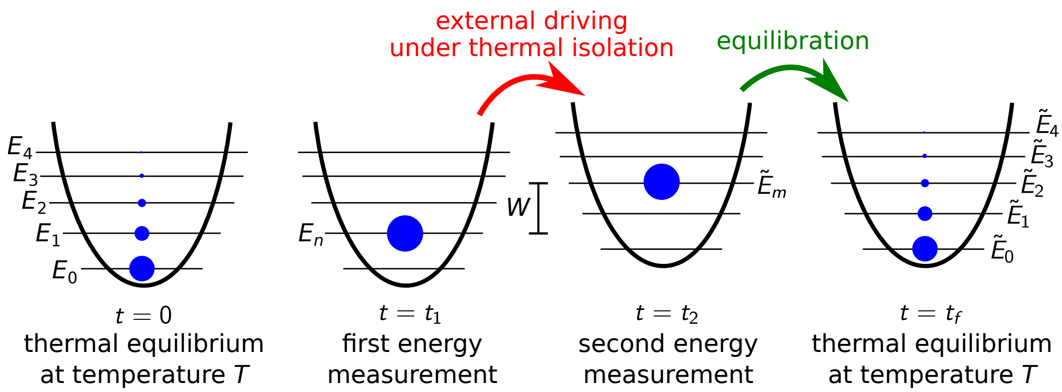
PHYS 414 Problem Set 5: Quantum Jarzynski equality and decoherence

Problem 1: Quantum Jarzynski equality



In a recent experimental breakthrough, Kihwan Kim and collaborators were able to directly measure the work required to drive a quantum system (a $^{171}\mathrm{Yb}^+$ ion trapped in a harmonic potential) between two different equilibrium states [An *et al.*, Nature Physics **11**, 193 (2015)]. For the first time, researchers could directly study fundamental thermodynamic relationships between work and free energy at the quantum scale.

The experimental protocol, illustrated above, is as follows:

1. At $t = 0$, we have a quantum system with Hamiltonian $\mathcal{H}$ at thermal equilibrium with temperature T. Let us denote the eigenstates of $\mathcal{H}$ by $|n\rangle$, with $n = 0, 1, 2, \ldots$, and the corresponding eigenvalues E_n. The system remains in equilibrium until $t = t_1$.

2. At $t = t_1$ the experimentalist performs an energy measurement on the system, and the result is E_n for some n.

3. For $t_1 < t < t_2$, the system is thermally isolated, so it cannot exchange heat with its environment. The experimentalist now varies the Hamiltonian in some time-dependent manner. The net result is that the system evolves during this period according to a unitary operator $\mathcal{U}$, satisfying $\mathcal{U}^\dagger\mathcal{U} = \mathcal{U}\mathcal{U}^\dagger = I$. In other words, if $|\psi(t_1)\rangle$ was the state of the system at time t_1, then $|\psi(t_2)\rangle = \mathcal{U}|\psi(t_1)\rangle$. At $t = t_2$, at the end of this driving process, the system has a new Hamiltonian, $\tilde{\mathcal{H}}$, with eigenstates $|\tilde{m}\rangle$ and energies $\tilde{E}_m$.

4. At $t = t_2$ the experimentalist again performs an energy measurement, and the result is $\tilde{E}_m$ for some m. We define $W = \tilde{E}_m - E_n$ as the net amount of work done on the system. Note that W can be positive or negative.

5. For $t > t_2$, the system continues to have Hamiltonian $\tilde{\mathcal{H}}$. It is coupled back to the environment, and allowed to reach equilibrium at the same temperature T as before. At the final time $t = t_f$ it is again in thermal equilibrium.

Note that every time the experiment is run, it will potentially record a different value of W, since the measured energies E_n and $\tilde{E}_m$ in steps 2 and 4 may be different. Thus if you redo the experiment many times, you can construct a probability distribution of work values $P(W)$. On the other hand, the difference in Helmholtz free energies, $\Delta F = F_f - F_0$, between the equilibrium states at $t = t_f$ and $t = 0$, is always the same for every run. In classical thermodynamics for macroscopic systems, the second law implies that $W \geq \Delta F$. Let us see what happens in the quantum case.

Useful theorem: Jensen's inequality states that $e^{\langle x \rangle} \leq \langle e^x \rangle$, where the $\langle\ \rangle$ brackets denote an average with respect to some probability distribution of x.

a) Write expressions for the partition functions Z_0 and Z_f of the system at the beginning and end of the experiment ($t = 0$ and $t = t_f$). Assume Boltzmann thermal equilibrium.

b) Write an expression for the Helmholtz free energy difference $\Delta F = F_f - F_0$ in terms of Z_f and Z_0?

c) What is the probability $P(n)$ that in any given experimental run, you measure the energy value E_n in step 2?

d) What is the transition probability $P(m|n)$, defined as the probability of finding $\tilde{E}_m$ in step 4, assuming the result of step 2 was E_n?

The work distribution $P(W)$ can now be written as:

$$P(W) = \sum_{m,n} \delta(W - \tilde{E}_m + E_n) P(m|n) P(n)$$

The Dirac delta enforces the fact that the only allowed values for W correspond to differences between the energy levels of $\tilde{\mathcal{H}}$ and $\mathcal{H}$.

e) Calculate the average $\langle \exp(-\beta W) \rangle = \int_{-\infty}^{\infty} dW\, P(W) \exp(-\beta W)$, where $\beta = 1/k_B T$. Prove the identity $\langle \exp(-\beta W) \rangle = \exp(-\beta \Delta F)$.

This remarkable identity—known as the quantum Jarzynski equality—is valid for all possible ways of driving the system in Step 3 (all possible unitary operators $\mathcal{U}$). It was first derived independently by Hal Tasaki and Jorge Kurchan in 2000, three years after the same identity was introduced by Christopher Jarzynski for classical systems. Experimental verification was only achieved in 2015 with the Kim group ion trapping study.

f) Show that the identity in part e) implies the inequality $\langle W \rangle \geq \Delta F$. Thus the second law of thermodynamics is valid in this quantum context, but defined in terms of the mean work $\langle W \rangle$.

g) The result of part f) leaves open the possibility that for some experimental runs you might find $W < \Delta F$, a quantum "violation" of the second law, which can still be consistent with the overall average $\langle W \rangle \geq \Delta F$. To see if this can happen, let us consider the simple case where both $\mathcal{H}$ and $\tilde{\mathcal{H}}$ are two-level systems, with energies E_0, $E_1 = E_0 + \mu$ for $\mathcal{H}$, and $\tilde{E}_0 = E_0 + \nu$, $\tilde{E}_1 = E_0 + \nu + \mu$ for $\tilde{\mathcal{H}}$. Here μ and ν are constants, with $\mu > 0$. In this two level case, the most general unitary operator $\mathcal{U}$ can be written as a 2×2 matrix with elements:

$$\langle \tilde{0} | \mathcal{U} | 0 \rangle = a e^{i\phi}, \quad \langle \tilde{0} | \mathcal{U} | 1 \rangle = b e^{i\phi}, \quad \langle \tilde{1} | \mathcal{U} | 0 \rangle = -b^* e^{i\phi}, \quad \langle \tilde{1} | \mathcal{U} | 1 \rangle = a^* e^{i\phi},$$

where a and b are complex constants that satisfy $|a|^2 + |b|^2 = 1$, and ϕ is a real constant. Find the probability that an experimental run will have $W < \Delta F$.

As you can see from this result, in general the probability can be non-zero! But before you run off and try to build a perpetual motion machine, note that for large violations of the second law, $\Delta F - W \gg k_B T$, the probability that you will see such a violation vanishes exponentially. If you want to get a (big) free lunch, be prepared to wait a while.

Problem 2: Decoherence for imperfect measurements

In class we discussed how a quantum measurement on a system can be seen as one specific example of an interaction of a system with some external environment. Here we will generalize that idea to "imperfect" measurements, where we imagine that our environment acts like an error-prone measurement apparatus.

a) Let us imagine that at time t we have a qubit ensemble with some arbitrary density matrix $\hat{\rho}(t)$. The matrix elements of this operator in the basis $\{|0\rangle, |1\rangle\}$ are denoted as $\rho_{ij}(t) = \langle i|\hat{\rho}(t)|j\rangle$. Between time t and $t+\delta t$, the environment (apparatus) does a measurement projecting the system on the $\{|0\rangle, |1\rangle\}$ basis. Imagine the measurement was a traditional, perfect quantum measurement: if your apparatus output 0, the system state post-measurement would be $|0\rangle$, and if it output 1, the system state post-measurement would be $|1\rangle$. For a perfect apparatus, what is the probability of measuring 0, and what is the probability of measuring 1, in terms of $\rho_{ij}(t)$?

b) An imperfect apparatus is defined as follows. For an initial density matrix $\hat{\rho}(t)$ it measures 0 with the same probability derived above, but it occasionally messes up the wavefunction collapse: the system will be in the wrong state $|1\rangle$ post-measurement of 0 with small probability ϵ_{10}, and the correct state $|0\rangle$ with probability $1 - \epsilon_{10}$. Analogously the apparatus measures 1 with the same probability derived in part a, but results in the wrong system state $|0\rangle$ with probability ϵ_{01}, and the right state $|1\rangle$ with probability $1 - \epsilon_{01}$. Write down the density matrix $\hat{\rho}(t + \delta t)$ post-measurement. *Hint:* Remember post-measurement you are either in state $|0\rangle$ or $|1\rangle$. To find the corresponding density matrix $\hat{\rho}(t + \delta t)$, you need to know what fraction of your ensemble is in either state, given that you started pre-measurement with $\hat{\rho}(t)$.

c) Show that you can express your answer from part b in the form of a Kraus representation:

$$\hat{\rho}(t + \delta t) = \sum_{k=1}^{4} \hat{M}_k \hat{\rho}(t) \hat{M}_k^\dagger$$

Find the four Kraus operators $\hat{M}_k$, and verify that $\sum_k \hat{M}_k^\dagger \hat{M}_k = \hat{I}$, where $\hat{I}$ is the identity.

d) By writing the equation for $\hat{\rho}(t + \delta t)$ explicitly in terms of matrix elements in the $\{|0\rangle, |1\rangle\}$ basis, and dividing by δt, show that you can rearrange the results to look like a classical master equation for the diagonal elements:

$$\frac{d\rho_{00}(t)}{dt} = W_{01}\rho_{11}(tt) - W_{10}\rho_{00}(t)$$
$$\frac{d\rho_{11}(t)}{dt} = W_{10}\rho_{00}(tt) - W_{01}\rho_{11}(t)$$

where $d\rho_{ii}(t)/dt = (\rho_{ii}(t+\delta t) - \rho_{ii}(t))/\delta t$. Find expressions for the transition rates W_{ij}. Also show that $\rho_{01}(t+\delta t) = \rho_{10}(t+\delta t) = 0$, and hence the off-diagonal elements of $\hat{\rho}(t)$ are sent to zero after the imperfect measurement: a simple example of decoherence in action.