Aspects of quantum work and quantum heat

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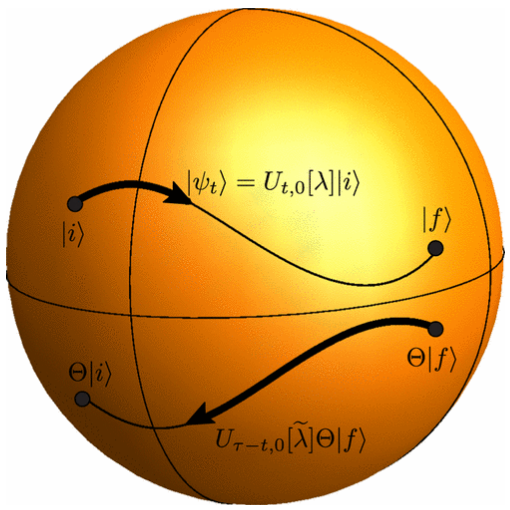

REVIEWS OF MODERN PHYSICS, VOLUME 83, JULY–SEPTEMBER 2011

Colloquium: Quantum fluctuation relations: Foundations and applications

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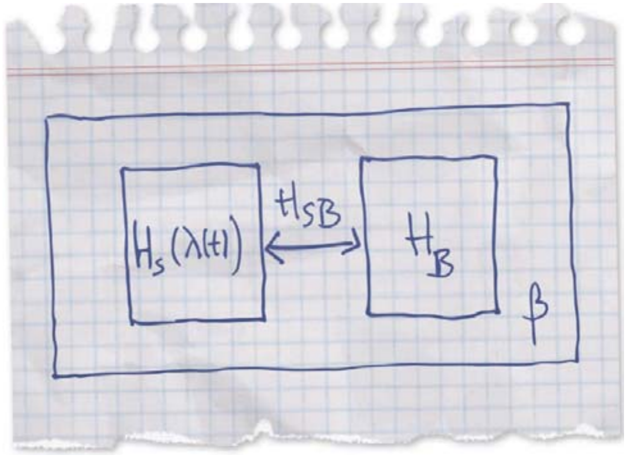
(Received 10 December 2010; published 6 July 2011)

P. Hänggi and P. Talkner, Nature Physics **11**, 108 -110 (2015)



PERSPECTIVE | INSIGHT

The other QFT

Peter Hänggi and Peter Talkner

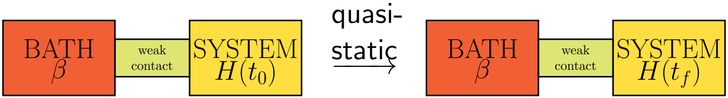
Fluctuation theorems go beyond the linear response regime to describe systems far from equilibrium. But what happens to these theorems when we enter the quantum realm? The answers, it seems, are now coming thick and fast.

Nonequilibrium aspects of work and heat fluctuations

Equilibrium versus nonequilibrium processes

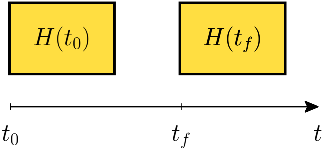
Isothermal quasistatic process:

$e^{-\beta H(t_0)}/Z(t_0)$ $\qquad$ $e^{-\beta H(t_f)}/Z(t_f)$

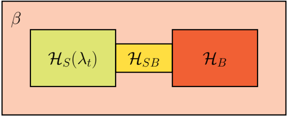


$$\Delta F = w = \langle w \rangle$$

Non-equilibrium process:



$p_{t_f,t_0}(w) = ?$ pdf of work



$$\mathcal{H}(\lambda_t) = \mathcal{H}_S(\lambda_t) + \mathcal{H}_B + \mathcal{H}_{SB}$$

$$\varrho(\lambda_0) = e^{-\beta \mathcal{H}(\lambda_0)} / Y(\lambda_0)$$

Protocols: role of time-dependence for work and heat (?)

Aspects of work fluctutions: classical case

INCLUSIVE VS. EXCLUSIVE VIEWPOINT

C. Jarzynski, C.R. Phys. 8 495 (2007)

$$H(\mathbf{z},\lambda_t) = H_0(\mathbf{z}) - \lambda_t Q(\mathbf{z})$$

$$\begin{aligned} W &= -\int dt Q_t \dot{\lambda}_t \\ &= H(\mathbf{z}_\tau,\lambda_\tau) - H(\mathbf{z}_0,\lambda_0) \end{aligned}$$

Not necessarily of the textbook form $\int \mathrm{d}$(displ.)$\times$ (force)

$$\begin{aligned} W_0 &= \int dt \lambda_t \dot{Q}_t \\ &= H_0(\mathbf{z}_\tau) - H_0(\mathbf{z}_0) \end{aligned} \qquad \dot{\mathbf{z}}_t = \{H(\mathbf{z}_t,\lambda_t);\mathbf{z}\}$$

G.N. Bochkov and Yu. E. Kuzovlev JETP **45**, 125 (1977)

GAUGE FREEDOM

$$
\begin{aligned}
H'(\mathbf{z}, t) &= H(\mathbf{z}, t) + g(t) \\
W' &= W + g(\tau) - g(0) \\
\Delta F' &= \Delta F + g(\tau) - g(0)
\end{aligned}
$$

$W, \Delta F$ are gauge dependent: **not true physical quantities**

WARNING: be consistent! use same gauge to calculate W and ΔF

$$
\langle e^{-\beta W'} \rangle = e^{-\beta \Delta F'} \iff \langle e^{-\beta W} \rangle = e^{-\beta \Delta F}
$$

The fluctuation theorem is gauge invariant !

Gauge: irrelevant for dynamics
crucial for ENERGY-HAMILTONIAN connection

GAUGE FREE vs. GAUGE DEPENDENT EXPRESSIONS OF CLASSICAL WORK

$$H' = H_0(\mathbf{z}) - \lambda_t Q(\mathbf{z}) + g(t)$$

Inclusive work:

$$W' = H'(\mathbf{z}_\tau, \tau) - H'(\mathbf{z}_0, 0) \quad , \quad g\text{-dependent}$$

$$W^{\text{phys}} = -\int \mathrm{d}t Q_t \dot{\lambda}_t \quad , \quad \cancel{g\text{-independent}}$$

$$W^{\text{phys}} = W' - g(\tau) + g(0)$$

Exclusive work:

$$W_0 = H_0(\mathbf{z}_\tau, \lambda_\tau) - H_0(\mathbf{z}_0, \lambda_0)$$

$$= \int \mathrm{d}t \lambda_t \dot{Q}_t \quad , \quad g\text{-independent}$$

Dissipated work:

$$W_{\text{diss}} = H'(\mathbf{z}_\tau, \tau) - H'(\mathbf{z}_0, 0) - \Delta F' \,, \qquad \text{g-independent}$$

INCLUSIVE, EXCLUSIVE and DISSIPATED WORK

$$W_{diss} = W - \Delta F \qquad \langle e^{-\beta W_{diss}} \rangle = 1$$

W, W_0, W_{diss} are DISTINCT stochastic quantities

$$p[x;\lambda] \neq p_0[x;\lambda] \neq p_{diss}[x;\lambda]$$

They coincide for cyclic protocols $\lambda_0 = \lambda_\tau$

M.Campisi, P. Talkner and P. Hänggi, Phil. Trans. R. Soc. A **369**, 291 (2011)

Work

Classical closed system:

$$
\begin{aligned}
w &= H(z(\tau), \lambda(\tau)) - H(z, \lambda(0)) \\
&= \int_0^\tau dt \, \frac{dH(z(t), \lambda(t))}{dt} \\
&= \int_0^\tau dt \, \frac{\partial H(z(t), \lambda(t))}{\partial \lambda} \dot{\lambda}(t)
\end{aligned}
$$

Note that a proper gauge must be used in order that the Hamiltonian yields the energy.

Work characterizes a process; it comprises information from states at distinct times. Hence it is not an observable.

The measurement of the quantum versions of power- and energy-based work definitions requires different strategies.

WORK IS NOT AN OBSERVABLE

P. Talkner et al. PRE 75 050102 (2007)

Work characterizes PROCESSES, not states!
(δW is not exact)

Work cannot be represented by a Hermitean operator $\mathcal{W}$

$W[\mathbf{z}_0; \lambda] \longrightarrow w = E_m^{\lambda_\tau} - E_n^{\lambda_0}$ two-measurements

$E_n^{\lambda_t}$ =instantaneous eigenvalue: $\mathcal{H}(\lambda_t)|\psi_n^{\lambda_t}\rangle = E_n^{\lambda_t}|\psi_n^{\lambda_t}\rangle$

Aspects of quantum work

Projective & generalized measurements

1. Two energy measurements:

One at the beginning, the other at the end of the protocol yield eigenvalues $e_n(0)$ and $e_m(\tau)$ of $H(\lambda(0))$ and $H(\lambda(\tau))$.

$$w^e = e_m(\tau) - e_n(0) \Longrightarrow \text{fluctuation theorems.}$$

2. Power-based work:

Requires a continuous measurement of power.

E.g. for $H(\lambda) = H_0 + \lambda Q$, a continuous observation of the generalized coordinate Q is required leading to a freezing of the systems dynamics in an eigenstate of Q.

$$w_N^p = \sum_{k=1}^{N} \dot{\lambda}(t_k) q_{\alpha_k} \frac{\tau}{N+1}\,, \quad Q = \sum_{\alpha} q_\alpha \Pi_\alpha^Q$$

Fluctuation theorems hold only if $[H_0, Q] = 0$ or equivalently $[H(\lambda(t)), H(\lambda(s))] = 0$ for all $t, s \in (0, \tau)$.

Hence the equivalence of the power- and energy-based work definitions for classical systems fails to hold in quantum mechanics.

3. “UNTOUCHED” WORK:

$$\langle w \rangle = \int dz[H(z(t),\lambda(t)) - H(z,\lambda(0))]\rho(z) \qquad \text{valid !}$$

$$\langle w \rangle = \mathrm{Tr}[H^H(\lambda(t)) - H(\lambda(0))]\rho(0) \qquad ????????$$

There is no operational definition of untouched work as a proper random variable.

With untouched work it would be possible to extract energy from quantum correlation and in particular from entanglement in multipartite systems.

A. Allahverdyan, Phys. Rev. E **90**, 032137 (2014).

K.V. Hovhannisyan, M. Perarnau-Llobet, M. Huber, A. Acín, Phys. Rev. Lett. **111**, 240401 (2013).

$$
\begin{aligned}
\mathcal{W}[\lambda] &= U_{t,0}^{\dagger}[\lambda]\mathcal{H}(\lambda_t)U_{t,0}[\lambda] - \mathcal{H}(\lambda_0) \\
&= \mathcal{H}_t^H(\lambda_t) - \mathcal{H}(\lambda_0) \\
&= \int_0^t \mathrm{d}t\dot{\lambda}_t \frac{\partial \mathcal{H}_t^H(\lambda_t)}{\partial \lambda_t}
\end{aligned}
$$

projective energy measurements

Probability of work

$$H(t)\varphi_{n,\lambda}(t) = e_n(t)\varphi_{n,\lambda}(t)$$

$$P_n(t) = \sum_\lambda |\varphi_{n,\lambda}(t)\rangle\langle\varphi_{n,\lambda}(t)|$$

$$\begin{aligned}
p_n &= \mathrm{Tr}\ P_n(t_0)\rho(t_0) \\
&= \text{probability of being at energy } e_n(t_0) \text{ at } t = t_0 \\
\\
\rho_n &= P_n(t_0)\rho(t_0)P_n(t_0)/p_n \\
&= \text{state after measurement} \\
\\
\rho_n(t_f) &= U_{t_f,t_0}\rho_n U^+_{t_f,t_0} \\
\\
p(m|n) &= \mathrm{Tr} P_m(t_f)\rho_n(t_f) \\
&= \text{conditional probability of getting to energy } e_m(t_f)
\end{aligned}$$

Probability of work

$$\boxed{p_{t_f,t_0}(w) = \sum_{n,m} \delta(w - [e_m(t_f) - e_n(t_0)])p(m|n)p_n}$$

Characteristic function of work

$$
\begin{aligned}
G_{t_f,t_0}(u) &= \int dw\, e^{iuw} p_{t_f,t_0}(w) \\
&= \sum_{m,n} e^{iue_m(t_f)} e^{-iue_n(t_0)} \mathrm{Tr} P_m(t_f) U_{t_f,t_0} \rho_n U^{+}_{t_f,t_0} p_n \\
&= \sum_{m,n} \mathrm{Tr} e^{iuH(t_f)} P_m(t_f) U_{t_f,t_0} e^{-iH(t_0)} \rho_n U^{+}_{t_f,t_0} p_n \\
&= \mathrm{Tr} e^{iuH_H(t_f)} e^{-iuH(t_0)} \bar{\rho}(t_0) \\
&\equiv \langle e^{iuH(t_f)} e^{-iuH(t_0)} \rangle_{t_0}
\end{aligned}
$$

$$H_H(t_f) = U^{\dagger}_{t_f,t_0} H(t_f) U_{t_f,t_0},$$

$$\bar{\rho}(t_0) = \sum_n P_n(t_0)\rho(t_0)P_n(t_0), \quad \bar{\rho}(t_0) = \rho(t_0) \iff [\rho(t_0), H(t_0)]$$

P. Talkner, P. Hänggi, M. Morillo, Phys. Rev. E **77**, 051131 (2008)
P.Talkner, E. Lutz, P. Hänggi, Phys. Rev. E **75**, 050102(R) (2007)

Choose $u = i\beta$

$$\begin{aligned}
\langle e^{-\beta w} \rangle &= \int dw\; e^{-\beta w} p_{t_f,t_0}(w) \\
&= G^c_{t_f,t_0}(i\beta) \\
&= \mathrm{Tr} e^{-\beta H_H(t_f)} e^{\beta H(t_0)} Z^{-1}(t_0) e^{-\beta H(t_0)} \\
&= \mathrm{Tr} e^{-\beta H(t_f)} / Z(t_0) \\
&= Z(t_f)/Z(t_0) \\
&= e^{-\beta \Delta F}
\end{aligned}$$

quantum Jarzynski equality

Erratum: *Colloquium*: Quantum fluctuation relations: Foundations and applications [Rev. Mod. Phys. 83, 771 (2011)]

Michele Campisi, Peter Hänggi, and Peter Talkner

(published 19 December 2011)

DOI: 10.1103/RevModPhys.83.1653 PACS numbers: 05.30.−d, 05.40.−a, 05.60.Gg, 05.70.Ln, 99.10.Cd

The first line of Eq. (51) contains some typos: it correctly reads

$$G[u;\lambda] = \mathrm{Tr}\,\mathcal{T} e^{iu[\mathcal{H}_\tau^H(\lambda_\tau) - \mathcal{H}(\lambda_0)]} e^{-\beta\mathcal{H}(\lambda_0)}/Z(\lambda_0). \tag{51}$$

This compares with its classical analog, i.e., the second line of Eq. (27).

Quite surprisingly, notwithstanding the identity

$$\mathcal{H}_\tau^H(\lambda_\tau) - \mathcal{H}(\lambda_0) = \int_0^\tau dt\dot{\lambda}_t \frac{\partial \mathcal{H}_t^H(\lambda_t)}{\partial \lambda_t}, \tag{1}$$

one finds that generally

$$\mathcal{T} e^{iu[\mathcal{H}_\tau^H(\lambda_\tau) - \mathcal{H}(\lambda_0)]} \neq \mathcal{T} \exp\left[iu \int_0^\tau dt\dot{\lambda}_t \frac{\partial \mathcal{H}_t^H(\lambda_t)}{\partial \lambda_t}\right]. \tag{2}$$

≠ !

"=" IS WRONG

As a consequence, it is not allowed to replace $\mathcal{H}_\tau^H(\lambda_\tau) - \mathcal{H}(\lambda_0)$, with $\int_0^\tau dt\dot{\lambda}_t \partial \mathcal{H}_t^H(\lambda_t)/\partial\lambda_t$ in Eq. (51). Thus, there is no quantum analog of the classical expression in the third line of Eq. (27). This is yet another indication that "work is not an observable" (Talkner, Lutz, and Hänggi, 2007)). This observation also corrects the second line of Eq. (4) of the original reference (Talkner, Lutz, and Hänggi, 2007).

The correct expression is obtained from the general formula

$$\mathcal{T} \exp[A(\tau) - A(0)] = \mathcal{T} \exp\left[\int_0^\tau dt\left(\frac{d}{dt} e^{A(t)}\right) e^{-A(t)}\right], \tag{3}$$

where $A(t)$ is any time dependent operator [in our case $A(t) = iu\mathcal{H}_t^H(\lambda_t)$]. Equation (3) can be proved by demonstrating that the operator expressions on either side of Eq. (3) obey the same differential equation with the identity operator as the initial condition. This can be accomplished by using the operator identity $de^{A(t)}/dt = \int_0^1 ds e^{sA(t)} \dot{A}(t) e^{(1-s)A(t)}$.

There are also a few minor misprints: (i) The symbol ds in the integral appearing in the first line of Eq. (55) should read dt. (ii) The correct year of the reference (Morikuni and Tasaki, 2010) is 2011 (not 2010).

The authors are grateful to Professor Yu. E. Kuzovlev for providing them with this insight, and for pointing out the error in the second line of Eq. (51).

REFERENCES

Talkner P., E. Lutz, and P. Hänggi, 2007, Phys. Rev. E 75, 050102(R).

3. “UNTOUCHED” WORK:

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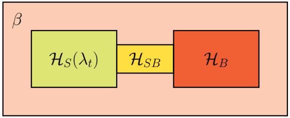
A. Allahverdyan, Phys. Rev. E **90**, 032137 (2014).

K.V. Hovhannisyan, M. Perarnau-Llobet, M. Huber, A. Acín, Phys. Rev. Lett. **111**, 240401 (2013).

OPEN SYSTEMS

$$H(\lambda(t)) \longrightarrow H_{SYSTEM}(\lambda(t)) + H_{BATH} + H_{S\text{-}B}$$

OPEN QUANTUM SYSTEM: WEAK COUPLING



$$\mathcal{H}(\lambda_t) = \mathcal{H}_S(\lambda_t) + \mathcal{H}_B + \mathcal{H}_{SB}$$

$$\varrho(\lambda_0) = e^{-\beta \mathcal{H}(\lambda_0)} / Y(\lambda_0)$$

$$\Delta E = E_m^{\lambda_\tau} - E_n^{\lambda_0} \qquad \text{system energy change}$$

$$\Delta E^B = E_\mu^B - E_\nu^B = -Q \qquad \text{bath energy change}$$

$$p[\Delta E, Q; \lambda] = \sum_{m,n,\mu,\nu} \delta[\Delta E - E_m^{\lambda_\tau} + E_n^{\lambda_0}] \delta[Q + E_\mu^B - E_\nu^B] p_{m\mu|n\nu}[\lambda] p_{n\nu}^0$$

$$\frac{p[\Delta E, Q; \lambda]}{p[-\Delta E, -Q; \widetilde{\lambda}]} = e^{\beta(\Delta E - Q - \Delta F_S)} \qquad \Delta F_S = -\beta^{-1} \ln \frac{\mathcal{Z}_S(\lambda_\tau)}{\mathcal{Z}_S(\lambda_0)}$$

$$\Delta E = w + Q \qquad \frac{p[w, Q; \lambda]}{p[-w, -Q; \widetilde{\lambda}]} = e^{\beta(w - \Delta F_S)}$$

P. Talkner, M. Campisi, P. Hänggi, J.Stat.Mech. (2009) P02025

$$\rho_0 = Z^{-1}(t_0)e^{-\beta\left(H^S(t_0)+H^{SB}+H^B\right)} \qquad \text{therm. eq. at } t_0$$

$$\approx \rho_0^0\left[1-\int_0^\beta d\beta' e^{\beta'\left(H^S(t_0)+H^B\right)}\delta H^{SB} e^{-\beta'\left(H^S(t_0)+H^B\right)}\right]$$

$$\rho_0^0 = Z_S^{-1}(t_0)Z_B^{-1}e^{-\beta\left(H^S(t_0)+H^B\right)}$$

$$\bar{\rho}_0 = \sum_{i,\alpha} P_{i,\alpha}(t_0)\rho_0 P_{i,\alpha}(t_0)$$

$$= \rho_0^0 + \mathcal{O}\left((\delta H^{SB})^2\right)$$

$$\boxed{G^{E,Q}_{t_f,t_0}(u,v) = \mathrm{Tr}\, e^{i\left(uH_H^S(t_f)-vH_H^B(t_f)\right)}e^{-i\left(uH^S(t_0)-vH^B\right)}\rho_0^0}$$

Crooks theorem for energy and heat

$$Z_S(t_0)\,G^{\Delta E,Q}_{t_f,t_0}(u,v) = Z_S(t_f)\,G^{\Delta E,Q}_{t_0,t_f}(-u+i\beta,-v-i\beta)$$

$$\boxed{\frac{p_{t_f,t_0}(\Delta E, Q)}{p_{t_0,t_f}(-\Delta E,-Q)} = \frac{Z_S(t_f)}{Z_S(t_0)}e^{\beta(\Delta E - Q)} = e^{-\beta(\Delta F_S - \Delta E + Q)}}$$

$$\Delta E = E_m^{\lambda_t} - E_n^{\lambda_0}$$

$$Q = -\Delta E^B = -E_\mu^B + E_\nu^B$$

$$w = \Delta E - Q : \qquad \text{work}$$

$$\boxed{\frac{p^{Q,w}_{t_f,t_0}(Q,w)}{p^{Q,w}_{t_0,t_f}(-Q,-w)} = e^{-\beta(\Delta F_S - w)}, \qquad \frac{p^{w}_{t_f,t_0}(w)}{p^{w}_{t_0,t_f}(-w)} = e^{-\beta(\Delta F_S - w)}}$$

$$\boxed{p_{t_f,t_0}(Q|w) = p_{t_0,t_f}(-Q|-w), \qquad p_{t_f,t_0}(Q|w) = \frac{p^{Q,w}_{t_f,t_0}(Q,w)}{p^{w}_{t_f,t_0}(w)}}$$

P. Talkner, M. Campisi, and P. Hänggi, J. Stat. Mech. (2009) P02025.

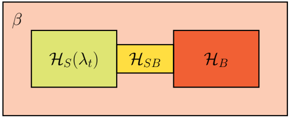
$$\frac{p_{t_f,t_0}(w|Q)}{p_{t_0,t_f}(-w|-Q)} = e^{\beta Q}\langle e^{-\beta w}|Q\rangle$$

$$\langle e^{\beta Q}\rangle = \frac{\mathrm{Tr} e^{-\beta H^S(t_0)} e^{-\beta H_H^B(t_f)}}{Z_S(t_0) Z_B}$$

$$\langle e^{-\beta E}\rangle = \frac{\mathrm{Tr} e^{-\beta H_H^S(t_f)} e^{-\beta H^B}}{Z_S(t_0) Z_B}$$

P. Talkner, M. Campisi and P. Hänggi, J. Stat. Mech. Theor. Exp. P02025 (2009).

OPEN QUANTUM SYSTEM: STRONG COUPLING



$$H(\lambda_t) = H_S(\lambda_t) + H_{SB} + H_B$$

$$w = \mathcal{E}_m^{\lambda_\tau} - \mathcal{E}_n^{\lambda_0} = \text{work on total system=work on } \mathcal{S}$$

$$Y(\lambda_t) = \mathrm{Tr} e^{-\beta H(\lambda_t)} = \text{partition function of total system}$$

$$\mathcal{Z}_S(\lambda_t) = \frac{Y(\lambda_t)}{\mathcal{Z}_B} \neq \mathrm{Tr}_S e^{-\beta \mathcal{H}_S(\lambda_t)} = \text{partition function of } \mathcal{S}$$

$$F_S(\lambda_t) = -\beta^{-1} \ln \mathcal{Z}_S(\lambda_t) \text{ proper free energy of open system}$$

$$\frac{p[w;\lambda]}{p[-w;\widetilde{\lambda}]} = \frac{Y(\lambda_\tau)}{Y(\lambda_0)} e^{\beta w} = \frac{\mathcal{Z}(\lambda_\tau)}{\mathcal{Z}(\lambda_0)} e^{\beta w} = e^{\beta(w - \Delta F_S)}$$

M. Campisi, P. Talkner, and P. Hänggi, Phys. Rev. Lett. **102** 210401 (2009)

Free energy of a system strongly coupled to an environment

Thermodynamic argument:

$$F_S = F - F_B^0$$

F total system free energy
F_B bare bath free energy.

With this form of free energy the three laws of thermodynamics are fulfilled.

G.W. Ford, J.T. Lewis, R.F. O'Connell, Phys. Rev. Lett. **55**, 2273 (1985);
P. Hänggi, G.L. Ingold, P. Talkner, New J. Phys. **10**,115008 (2008);
G.L. Ingold, P. Hänggi, P. Talkner, Phys. Rev. E **79**, 0611505 (2009).

Partition function

$$\mathbf{Z_S(t) = \frac{Y(t)}{Z_B}}$$

where $\quad Z_B = \mathrm{Tr}_B e^{-\beta H_B}$

Main results

$$\frac{p_{t_f,t_0}(w)}{p_{t_0,t_f}(-w)} = e^{\beta w}\frac{Y(t_f)}{Y(t_0)} = e^{\beta w}\frac{Z_S(t_f)}{Z_S(t_0)} = e^{\beta(w-\Delta F_S)}$$

$$\langle e^{-\beta w}\rangle = e^{-\beta \Delta F_S}$$

Quantum Hamiltonian of Mean Force

$$Z_S(t) := \frac{Y(t)}{Z_B} = \mathrm{Tr}_S\, e^{-\beta H^*(t)}$$

where

$$H^*(t) := -\frac{1}{\beta} \ln \frac{\mathrm{Tr}_B\, e^{-\beta(H_S(t)+H_{SB}+H_B)}}{\mathrm{Tr}_B\, e^{-\beta H_B}}$$

also

$$\frac{e^{-\beta H^*(t)}}{Z_S(t)} = \frac{\mathrm{Tr}_B\, e^{-\beta H(t)}}{Y(t)}$$

M. Campisi, P. Talkner, P. Hänggi, Phys. Rev. Lett. **102**, 210401 (2009).

PHYSICAL REVIEW E **93**, 022131 (2016)

Aspects of quantum work

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[2]*Institute of Physics, University of Silesia, 40007 Katowice, Poland*
[3]*Nanosystems Initiative Munich, Schellingstrasse 4, D-80799 München, Germany*
(Received 8 December 2015; published 23 February 2016)

Various approaches of defining and determining work performed on a quantum system are compared. Any operational definition of work, however, must allow for two facts: first, that work characterizes a process rather than an instantaneous state of a system and, second, that quantum systems are sensitive to the interactions with a measurement apparatus. We compare different measurement scenarios on the basis of the resulting postmeasurement states and the according probabilities for finding a particular work value. In particular, we analyze a recently proposed work meter for the case of a Gaussian pointer state and compare it with the results obtained by two projective and, alternatively, two Gaussian measurements. In the limit of a strong effective measurement strength the work distribution of projective two energy measurements can be recovered. In the opposite limit the average of work becomes independent of any measurement. Yet the fluctuations about this value diverge. The performance of the work meter is illustrated by the example of a spin in a suddenly changing magnetic field.

generalized energy measurements

Generalized energy measurements

Positive operator valued measures (POVM) as generalized measurements

projective	POVM	
Π_n	$M_n,\ M_n^\dagger$	measurement operators
$\sum_n \Pi_n \rho \Pi_n$	$\sum_n M_n \rho M_n^\dagger$	ρ_{pm}: unselectice pm state
$\mathrm{Tr} \Pi_n \rho \Pi_n$	$\mathrm{Tr} M_n \rho M_n^\dagger$	$p_n = \mathrm{Prob}(n \text{ in } \rho)$
$\Pi_n \rho \Pi_n / p_n$	$\rho_n = M_n \rho M_n^\dagger / p_n$	ρ_n: selective pm state
$\sum_n \Pi_n = \mathbb{1}$	$\sum_n M_n^\dagger M_n = \mathbb{1}$	normalization

measurement error:

$$p(n|m) = \mathrm{Tr} M_n \Pi_m M_n^\dagger / \mathrm{Tr} \Pi_m = \mathrm{Tr} M_n^\dagger M_n \Pi_m / \mathrm{Tr} \Pi_m$$

A measurement is ERROR-FREE if

$$p(n|m) = \delta_{n,m}$$

Generalized measurements

In QM the measurement of an observable $\mathcal{A}$ in a state ρ

(i) assigns to $\mathcal{A}$ a real value a with probability p_a

(ii) transforms the state ρ of the system at the instant before the measurement to a new state after the measurement:

$$\rho_a^{pm} = \phi_a(\rho)/p_a$$

The *measurement operation* $\phi_a : TC(\mathcal{H}) \to TC(\mathcal{H})$ is a linear, positive and contractive map.

Hence it can be represented as (K. Kraus, *States, Effects and Operators*, Springer 1983)

$$\phi_a(\rho) = \sum_\alpha M_\alpha^a \rho M_\alpha^{a\dagger} \,, \quad M_\alpha^a \in B(\mathcal{H}) : \quad \text{Kraus operators}$$

$$p_a = \mathrm{Tr}\phi_a(\rho) : \qquad \text{probability to find } a$$

$$\rho(t^+) = \sum_a \rho_a^{pm} p_a = \sum_a \phi_a(\rho(t)) \ : \quad \text{non-selective pm state}$$

Generalized measurement of work

Work is not an observable, hence it cannot be measured by a projective measurement but by a generalized measurement.
Based on two projective energy measurements the measurement of work w is determined by the operation

$$\phi_w(\rho(0)) = \sum_{m,n} \delta(w - e_m(\tau) + e_n(0)) \Pi_m(\tau) U_\Lambda \Pi_n(0) \rho(0) \Pi_n(0) U_\Lambda^\dagger \Pi_m(\tau)$$

Non-selective post-measurement state

$$\rho(0^+) = \sum_{m,n} \Pi_m(\tau) U_\Lambda \Pi_n(0) \rho(0) \Pi_n(0) U_\Lambda^\dagger \Pi_m(\tau)$$

Work statistics with generalized measurements

$\Lambda = \{\lambda(t)|0 \leq t \leq \tau\}, \qquad H(\lambda(t)) = \sum_n e_n(t)\Pi_n(t)$

When the state of the system is inquired with measurement operators $M_n(t)$, the joint probability of finding initially n and at the end of the protocol m is given by

$$p_\Lambda(m,n) = \mathrm{Tr} M_m(\tau) U(\Lambda) M_n(0) \rho(0)_\Lambda M_n^\dagger(0) U^\dagger(\Lambda) M_m^\dagger(\tau)$$

The pdf of work:

$$p_\Lambda(w) = \sum_{n,m} \delta(w - e_m(\tau) + e_n(0)) p_\Lambda(m,n)$$

The characteristic function:

$$G_\Lambda(u) = Z^{-1}(0) \mathrm{Tr} U^\dagger(\Lambda) Q(u,\tau) U(\Lambda) R(u,0)$$

$$G_\Lambda(u) = Z^{-1}(0)\mathrm{Tr}U^\dagger(\Lambda)Q(u,\tau)U(\Lambda)R(u,0)$$

$$Q(u,t) = \sum_m e^{iue_m(t)} M_m^\dagger(t) M_m(t)$$

$$R(u,t) = \sum_n e^{-iue_n(t)} M_n(t) e^{-\beta H(\lambda(t))} M_n^\dagger(t)$$

The Crooks relation holds iff

$$\mathrm{Tr}U^\dagger(\Lambda)Q(u,\tau)U(\Lambda)R(u,0) = \mathrm{Tr}U^\dagger(\Lambda)R(-u+i\beta)U(\Lambda)Q(-u+i\beta,0)$$

Condition on the measurement operators $M_n(t)$, $t = 0, \tau$.

Universal measurements

A universal energy measurement operator $M_n(t)$ identifies the eigenstate $|n,t\rangle$ of $H(\lambda(t))$, $t=0,\tau$. Further, it is independent of

(i) the protocol Λ
(ii) eigenvalues $e_k(0)$ and $e_k(\tau)$
(iii) the inverse temperature β

Choose as protocol:

$$H(\lambda(0)) \overset{\text{suddenly at } t=0^+}{\Longrightarrow} G\eta/\tau \overset{\text{suddenly at } t=\tau^-}{\Longrightarrow} H(\lambda(\tau))$$

G: arbitrary Hamiltonian, $\eta \geq 0$,
then $U(\Lambda) = e^{-iG\eta/\hbar}$ can become any unitary operator.

$$\mathrm{Tr}\, U^\dagger(\Lambda) Q(u,\tau) U(\Lambda) R(u,0) = \mathrm{Tr}\, U^\dagger(\Lambda) R(-u+i\beta,\tau) U(\Lambda) Q(-u+i\beta,0)$$

for all unitary $U(\Lambda)$ implies for universal measurements (i)

$$Q(u,t) = R(-u+i\beta,t) \quad t=0,\tau$$

$$\sum_m e^{iue_m(t)} \underbrace{\left[M_m^\dagger(t) M_m(t) - \sum_k e^{\beta(e_m(t)-e_k(t))} \overbrace{M_m(t)\Pi_k(t)M_m^\dagger(t)}^{\propto \delta_{m,k} \text{ because of (iii)}} \right]}_{=0 \text{ because of (ii)}} = 0$$

hence, (a) for $m \neq k$

$$p(m|k) = \mathrm{Tr} M_m(t)\Pi_k M_m^\dagger = 0$$

therefore $M_n(t)$ is an error-free measurement and thus $M_n(t) = |\psi_n(t)\rangle\langle n; t|$. (b) the $m = k$ terms yield

$$\underbrace{M_m^\dagger(t) M_m(t)}_{|m;t\rangle\langle\psi_m(t)|\psi_m(t)\rangle\langle m;t|} = \underbrace{M_m(t)\Pi_m(t)M_m^\dagger(t)}_{|\psi_m(t)\rangle\langle m;t|m;t\rangle\langle\psi_m(t)}$$

yields $|\psi_n(t)\rangle = |n; t\rangle$ and hence

$$M_n(t) = \Pi_n(t)\,, \quad t = 0, \tau$$

The Crooks relation holds for universal energy measurement operators only if they are projective.

Quantum Jarzynski equality

The Jarzynski equality holds for systems with infinite-dimensional Hilbert space and for universal measurement operators iff

(i) $M_n(0)$ is error-free $(p(n'|n) = \delta_{n',n})$, $M_n(0) = |\psi_n(0)\rangle\langle n;0|$

(ii) $\{|\psi_n(0)\rangle\}$ form a complete orthonormal basis, i.e. $\langle\psi_n(0)|\psi_k(0)\rangle = \delta_{n,k}$ and $\sum_n |\psi_n\rangle\langle\psi_n| = \mathbb{1}$

(iii) $\mathrm{Tr} M_m^\dagger(\tau) M_m(\tau) = 1$

P. Hänggi and P. Talkner, Nature Phys. **11**, 108 (2015).

Measurements during the protocol

Measurements of arbitrary observables during the force protocol lead to modified work distributions which still obey the Crooks relation as long as the corresponding measurement operators $\tilde{M}_x$ of the time reversed process are determined by the time-reversed adjoint measurement operators M_x forward process.

$$\tilde{M}_x = \theta M_x^\dagger \theta^\dagger$$

This implies that the measurement operators generate unital maps,

$$\sum_x M_x M_x^\dagger = \mathbb{1}$$

which also is necessary and sufficient for the Jarzynski equality to hold.

M. Campisi, P. Talkner, P. Hänggi, Phys. Rev. Lett. **102**, 210401 (2009).

G. Watanabe, B.P. Venkatesh, P. Talkner, M.Campisi, P. Hänggi, Phys. Rev. E **89**, 032114 (2014).

Continuous energy measurements

Gaussian energy measurement

$$M_E(t) = \frac{1}{(2\pi\mu^2)^{1/4}} \exp\left(\frac{1}{4\mu^2}(H(\lambda(t)) - E)^2\right)$$
$$M_E^\dagger(t) = M_E(t)$$

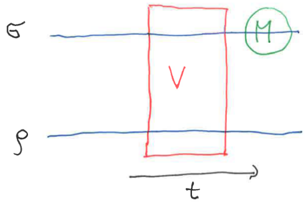
Gaussian failure distribution:

$$\begin{aligned} p_t(E|n) &= \mathrm{Tr} M_E^2(t)\Pi_n(t) \\ &= \frac{1}{\sqrt{2\pi\mu^2}} \exp\left(\frac{1}{2\mu^2}(e_n(t) - E)^2\right) \end{aligned}$$

with variance μ^2 which is independent of n.
Pdf to find the energy E' at the end of the protocol Λ conditioned on E in the beginning

$$P_\Lambda(E'|E) = \mathrm{Tr} M_{E'}^2(\tau) U(\Lambda) M_E(0) \rho_\Lambda M_E(0) U^\dagger(\Lambda)$$

von Neumann model of generalized energy measurement



$\rho \otimes \sigma$: initial state of system and pointer
$V = e^{-i\kappa HP/\hbar}$: system-pointer interaction
$H = \sum_n \epsilon_n \Pi_n$: system Hamiltonian
P: pointer-momentum, conjugate to pointer-position X
M: projective measurement of the pointer-position X

$$\phi_x(\rho) = \mathrm{Tr}_P \mathbb{Q}_x V \rho \otimes \sigma V^\dagger \qquad \text{operation}$$

$$= \sum_{n,n'} \sigma(x - \kappa e_n, x - \kappa e_{n'}) \Pi_n \rho \Pi_{n'}$$

$$\sigma(x, y) = \langle x|\sigma|y\rangle$$

$$\rho_x = \phi_x(\rho)/p^{(1)}(x) \qquad \text{post-measurement state}$$

$$p^{(1)}(x) = \mathrm{Tr}_S \phi_x(\rho) \qquad \text{pdf to measure } x$$

$$= \sum_n \sigma(x - \kappa e_n, x - \kappa e_n) \mathrm{Tr}_S \Pi_n \rho$$

Work operation and pdf

$$\Phi_w^{(2)}(\rho(0)) = \int dE \Phi_{E+w}^{(\tau)}(U_\Lambda \Phi_E^{(0)}(\rho(0)) U_\Lambda^\dagger)$$

$$= \frac{1}{\sqrt{4\pi\sigma_e^2}} \sum_{\substack{m,m' \\ n,n'}} e^{-\frac{1}{2\sigma_{nd}^2}\left[(e_m(\tau)-e_{m'}(\tau))^2+(e_n(0)-e_m(0))^2\right]}$$

$$\times\ e^{-\frac{1}{4\sigma_e^2}\left[w-\frac{1}{2}(w_{m,n}+w_{m',n'})+i\frac{\langle\{X,P\}\rangle}{2\hbar}(w_{m,n}-w_{m',n'})\right]^2}$$

$$\times\ \Pi_m(\tau) U_\Lambda \Pi_n(0) \rho \Pi_{n'}(0) U_\Lambda^\dagger \Pi_{m'}(\tau)$$

$$p_\Lambda^{(2)}(w) = \frac{1}{\sqrt{4\pi\sigma_e^2}} \sum_{\substack{m \\ n,n'}} e^{-\frac{1}{2\sigma_{nd}^2}[e_n(0)-e_{n'}(0)]^2}$$

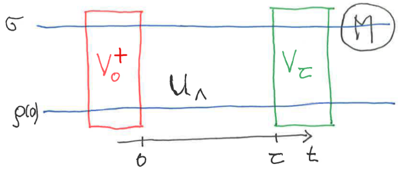
$$\times\ e^{-\frac{1}{4\sigma_e^2}\left[w-\frac{1}{2}(w_{m,n}+w_{m,n'})-i\frac{\langle\{X,P\}\rangle}{2\hbar}(e_n(0)-e_{n'}(0))\right]^2} p_\Lambda(m,n,n')$$

$$w_{m,n} = e_m(\tau) - e_n(0)$$

$$p_\lambda(m,n,n') = \mathrm{Tr}\Pi_m(\tau) U_\Lambda \Pi_n(0) \rho(0) \Pi_{n'}(0) U_\Lambda^\dagger \Pi_m(\tau)$$

Work meter

Device proposed by De Chiara, Roncaglia and Paz, (New J. Phys. **17**, 035004 (2015)) gives work by a single measurement.



$$V_0^\dagger = e^{i\kappa H(\lambda(0))P/\hbar}$$
$$V_\tau = e^{-i\kappa H(\lambda(\tau))P/\hbar}$$

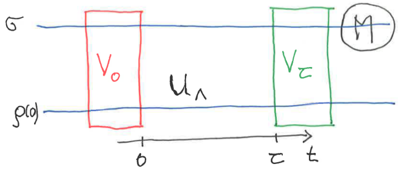
P: momentum conjugate to the pointer-position $X = \int dx\, x\, \mathbb{Q}_x$, $\mathbb{Q}_x = |x\rangle\langle x|$.

$$\phi_x^{wm}(\rho(0)) = \mathrm{Tr}_P \mathbb{Q}_x V_\tau U_\Lambda V_0^\dagger \rho(0) \otimes \sigma V_0 U_\Lambda^\dagger V_\tau^\dagger$$
$$= \sum_{\substack{m,m' \\ n,n'}} \sigma_0(x - \kappa w_{m,n}, x - \kappa w_{m,n'}) \Pi_m(\tau) U_\Lambda \Pi_n(0) \rho(0) \Pi_{n'}$$

$$\sigma_0(x,y) = \langle x|\sigma_0|y\rangle\ , \quad w_{m,n} = e_m(\tau) - e_n(0)$$

Work meter

Device proposed by De Chiara, Roncaglia and Paz, (New J. Phys. **17**, 035004 (2015)) gives work by a single measurement.



$$V_0 = e^{-i\kappa H(\lambda(0))P/\hbar}$$

$$V_\tau = e^{i\kappa H(\lambda(\tau))P/\hbar}$$

P: momentum conjugate to the pointer-position $X = \int dx\, x\, \mathbb{Q}_x$, $\mathbb{Q}_x = |x\rangle\langle x|$.

$$\phi_x^{wm}(\rho(0)) = \mathrm{Tr}_P \mathbb{Q}_x V_\tau U_\Lambda V_0 \rho(0) \otimes \sigma V_0^\dagger U_\Lambda^\dagger V_\tau^\dagger$$

$$= \sum_{\substack{m,m' \\ n,n'}} \sigma_0(x - \kappa w_{m,n}, x - \kappa w_{m,n'}) \Pi_m(\tau) U_\Lambda \Pi_n(0) \rho(0) \Pi_{n'}$$

$$\sigma_0(x,y) = \langle x|\sigma_0|y\rangle \;, \quad w_{m,n} = e_m(\tau) - e_n(0)$$

Gaussian work meter

For a Gaussian pointer and the calibration $x = \kappa w$ we obtain

$$\Phi_w^{wm}(\rho(0)) = \frac{1}{\sqrt{2\pi\sigma_e^2}} \sum_{\substack{m,m' \\ n,n'}} e^{-\frac{1}{2\sigma_{nd}^2}[w_{m,n}-w_{m',n'}]^2}$$

$$\times\ e^{-\frac{1}{2\sigma_e^2}\left[w-\frac{1}{2}(w_{m,n}+w_{m',n'})+i\frac{\langle\{X,P\}\rangle}{2\hbar}(w_{m,n}-w_{m',n'})\right]^2}$$

$$\times\ \Pi_m(\tau)U_\Lambda\Pi_n(0)\rho(0)\Pi_{n'}(0)U_\Lambda^\dagger\Pi_{m'}(\tau)$$

$$p_\Lambda^{wm}(w) = \frac{1}{\sqrt{2\pi\sigma_e^2}} \sum_{\substack{m \\ n,n'}} e^{-\frac{1}{2\sigma_{nd}^2}[e_n(0)-e_{n'}(0)]^2}$$

$$\times\ e^{-\frac{1}{2\sigma_e^2}\left[w-\frac{1}{2}(w_{m,n}+w_{m,n'})-i\frac{\langle\{X,P\}\rangle}{2\hbar}(e_n(0)-e_{n'}(0))\right]^2} p_\Lambda(m,n,n')$$

(2) accurate measurement: $\sigma_e^2 \to 0$

$$p_\Lambda^{wm}(w) = \sum_{\substack{m\\ n,n'}} \underbrace{e^{-\frac{1}{2\sigma^2{}_{nd}}[e_n(0)-e_{n'}(0)]^2}}_{\to \delta_{n,n'} \text{ for } \sigma_e^2 \to 0}$$

$$\times \underbrace{\frac{1}{\sqrt{2\pi\sigma_e^2}} e^{-\frac{1}{2\sigma_e^2}\left[w - e_m(\tau) + \frac{1}{2}(e_n(0)+e_{n'}(0)) - i\frac{\langle\{X,P\}\rangle}{2\hbar}(e_n(0)-e_{n'}(0))\right]^2}}_{\to \delta(w-e_m(\tau)+e_n(0)) \text{ for } \sigma_e^2 \to 0}$$

$$\times\, p_\Lambda(m,n,n')$$

With $\sigma_e^2 = \frac{\langle X^2\rangle}{\kappa^2} \to 0$ also $\sigma_{nd}^2 = \frac{\hbar^2}{\kappa^2\langle P^2\rangle} \to 0$; hence non-diagonal contributions with $n \neq n'$ are suppressed and the remaining Gaussian weights approach delta-functions.

$$p_\Lambda^{\text{pointer}}(w) \to p_\Lambda(w) \quad \text{for } \sigma_e^2 \to 0$$

(3) weak measurement $\sigma_{nd}^2 \to \infty$

$$p_\Lambda^{wm}(w) = \sum_{\substack{m\\ n,n'}} \frac{1}{\sqrt{2\pi\sigma_e^2}} \underbrace{e^{-\frac{1}{2\sigma_{nd}^2}[e_n(0)-e_{n'}(0)]^2}}_{\to 1 \text{ for } \sigma_{nd}^2 \to \infty}$$

$$\times\, e^{-\frac{1}{2\sigma_e^2}\left[w-\frac{1}{2}(w_{m,n}+w_{m,n'})-i\frac{\langle\{X,P\}\rangle}{2\hbar}(e_n(0)-e_{n'}(0))\right]^2} p_\Lambda(m,n,n')$$

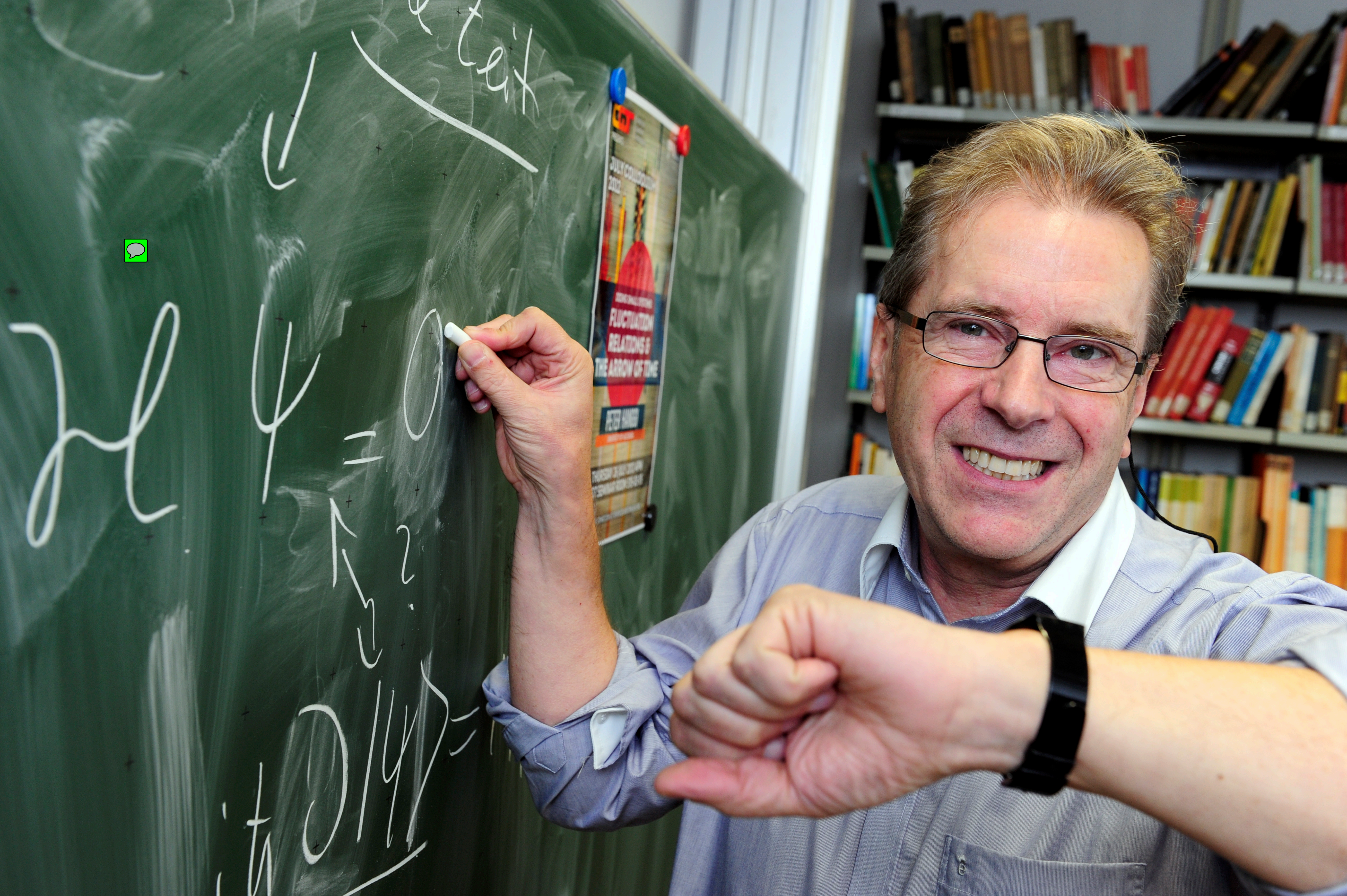
with $\sigma_{nd}^2 = \frac{\hbar^2}{\kappa^2\langle P^2\rangle} \to \infty$ also $\sigma_e^2 = \frac{\langle X^2\rangle}{\kappa^2} \to \infty$. In this limit $p_\Lambda^{wm}(w)$ becomes Gaussian with mean value

$$\langle W\rangle^{\text{weak}} = \mathrm{Tr} H(\lambda(\tau) U_\Lambda \rho(0) U_\Lambda^\dagger - \mathrm{Tr} H(\lambda(0))\rho(0)$$

and diverging variance σ_e^2.

In contrast, in the accurate limit one obtains

$$\langle W\rangle = \sum_n \mathrm{Tr} H(\lambda(\tau) U_\Lambda \Pi_n(0)\rho(0)\Pi_n(0) U_\Lambda^\dagger - \mathrm{Tr} H(\lambda(0))\rho(0)$$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RELATIONS &
THE ARROW OF TIME
PETER HANGGI

Conclusions

- Generalized energy measurements lead to work distributions which typically do not satisfy the Crooks relation relations.
- Exceptions are error-free measurements protocol-dependent post-measurement satisfying a detailed balance relation
- Imposing only the JE poses a weaker requirement: 1st set of measurements must be error-free with a complete orthogonal set of post-measurement states and second measurements must have with "effects" $M_n^\dagger(0)M_n(0)$ having unit trace.
- Continuous measurements with Gaussian measurement operators and constant variance obey modified fluctuation relations with protocol-independent modifications.
- Fluctuation relations continue to hold in presence of measurements during the force protocol under mild conditions on the measurement operators.

Conclusions

- Power-based work measurements do not yield meaningful results for quantum systems.
- For projective measurements the Crooks relation follows from generalized detailed balance which holds if (i) the initial state has Boltzmann-type diagonal matrix elements with respect to the eigen-basis of the initial Hamiltonian and (ii) the time-dependent Hamiltonian is time reversal invariant.
- Continuous measurements with Gaussian measurement operators and constant variance obey modified fluctuation relations with protocol-independent modifications.
- For a Gaussian pointer the De-Chiara-Roncaglia-Paz "work-meter" yields qualitatively same results as with a two Gaussian energy measurements but has higher precision. In the limit of accurate measurements it yields the results of projective energy measurements. In the weak limit it yields the average of "untouched" work, however, with divergent fluctuations.

ENDE

FIN

THAT'S IT

For non-degenerate energies, $\Pi_n = |n\rangle\langle n|$

$$M_n = \sum_{k,l} g^n_{k,l} |k\rangle\langle l|$$

with

$$p(n|m) = \sum_{n,k} |g_{k,m}|^2$$

M_n error-free:

$$M_n = |\psi_n\rangle\langle n|$$

where $|\psi_n\rangle$ is a pure post-measurement state. $\{|\psi_n\rangle\}$ need neither be orthogonal w.r.t. to different n, nor complete.

B.P. Venkatesh, G. Watanabe, P. Talkner, New J. Phys. **16**, 015032 (2014).

Work operation and pdf

$$\Phi_w^{(2)}(\rho(0)) = \int dE \Phi_{E+w}^{(\tau)}(U_\Lambda \Phi_E^{(0)}(\rho(0)) U_\Lambda^\dagger)$$

$$= \frac{1}{\sqrt{4\pi\sigma_e^2}} \sum_{\substack{m,m' \\ n,n'}} e^{-\frac{1}{2\sigma_{nd}^2}\left[(e_m(\tau)-e_{m'}(\tau))^2+(e_n(0)-e_m(0))^2\right]}$$

$$\times\ e^{-\frac{1}{4\sigma_e^2}\left[w-\frac{1}{2}(w_{m,n}+w_{m',n'})+i\frac{\langle\{X,P\}\rangle}{2\hbar}(w_{m,n}-w_{m',n'})\right]^2}$$

$$\times\ \Pi_m(\tau) U_\Lambda \Pi_n(0) \rho \Pi_{n'}(0) U_\Lambda^\dagger \Pi_{m'}(\tau)$$

$$p_\Lambda^{(2)}(w) = \frac{1}{\sqrt{4\pi\sigma_e^2}} \sum_{\substack{m \\ n,n'}} e^{-\frac{1}{2\sigma_{nd}^2}[e_n(0)-e_{n'}(0)]^2}$$

$$\times\ e^{-\frac{1}{4\sigma_e^2}\left[w-\frac{1}{2}(w_{m,n}+w_{m,n'})-i\frac{\langle\{X,P\}\rangle}{2\hbar}(e_n(0)-e_{n'}(0))\right]^2} p_\Lambda(m,n,n')$$

$$w_{m,n} = e_m(\tau) - e_n(0)$$

$$p_\lambda(m,n,n') = \mathrm{Tr}\Pi_m(\tau) U_\Lambda \Pi_n(0) \rho(0) \Pi_{n'}(0) U_\Lambda^\dagger \Pi_m(\tau)$$