Work Measurement as a Generalized Quantum Measurement

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We present a new method to measure the work w performed on a driven quantum system and to sample its probability distribution $P(w)$. The method is based on a simple fact that remained unnoticed until now: Work on a quantum system can be measured by performing a generalized quantum measurement at a single time. Such measurement, which technically speaking is denoted as a positive operator valued measure reduces to an ordinary projective measurement on an enlarged system. This observation not only demystifies work measurement but also suggests a new quantum algorithm to efficiently sample the distribution $P(w)$. This can be used, in combination with fluctuation theorems, to estimate free energies of quantum states on a quantum computer.

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Introduction.—For quantum systems the definition of work is rather subtle. As work is not represented by a Hermitian operator [1], it is not an ordinary quantum observable. Therefore, work measurement is certainly atypical. It is widely believed that work can only be measured by performing energy measurements at two times [1–4]. Instead, here we show that work can be measured at a single time by means of a very general class of quantum measurements which is denoted as a "positive operator valued measure" (or POVM) [5,6]. This type of generalized measurements is standard in quantum optics, quantum metrology, quantum information, etc. [5]. In fact, they define the most general set of questions to which quantum mechanics can assign probabilities. In general, they are such that (a) the number of outputs may be larger than the dimensionality of the space of states and (b) the states of the system after recording different outcomes of the measurement are not orthogonal. POVMs can always be realized as ordinary projective measurements on an enlarged system [5,6]. Thus, we show that, contrary to the common lore, work can be measured at a single time, that its probability distribution can be efficiently sampled, and that work is a magnitude with which other systems can directly couple.

Interest on work measurement in classical and quantum systems blossomed after the discovery of fluctuation theorems, the most significant result of statistical mechanics in decades [7,8]. Notably, Jarzynski identity establishes that for any nonequilibrium process, the probability $P(w)$ to detect work w contains the information required to compute free energy differences between equilibrium states. This has been used to evaluate free energies for classical systems at the nanoscale [9]. In the quantum regime, there have been proposals to determine $P(w)$ by measuring energy at two times with cold ions [10], to use properties of optical spectra to evaluate $P(w)$ [11], to perform many intermediate measurements on smaller subsystems [12], to adopt alternative strategies for driven two level systems [13], etc. Recently, the use of Ramsey interferometry has been suggested to estimate the characteristic function of $P(w)$ [14,15]. This method is based on the well-known scattering algorithm that estimates the average of any unitary operators [16]. This was later generalized for quantum open systems [17–19] and implemented in NMR experiments [20].

The method we present here is the only one that directly samples $P(w)$ by means of a projective measurement at a single time. By virtue of this fact, quantum coherence is destroyed only at that final time. Until then, the evolution is unitary. For this reason, this scheme can be used to study the role of quantum coherence in thermodynamical processes [21,22]. Our results helps to demystify work measurement for quantum systems. As we show, every value of work w can be coherently recorded in the state of a quantum register (an auxiliary system), which can then affect the fate of any other system, including the original one. Thus, although work is not represented by a Hermitian operator, it shares the essential properties of standard observables. Last, but not least, we show that our results motivate a novel quantum algorithm that, when executed in a quantum computer, would estimate free energies exploiting the efficient sampling of $P(w)$.

The nonexistence of a Hermitian work operator [1] is a consequence of the relation between work and energy differences. As the number of possible values of work $w = E_f - E_i$ is typically larger than the dimension of the space of states, a Hermitian operator representing work cannot exist. This does not imply that work is not measurable. Quite the opposite, work can be measured using the following strategy: Consider a system with initial state $\rho(t_0)$, which is driven from an initial Hamiltonian $H = H(t_i)$ to a final one $\tilde{H} = H(t_f)$. The results of energy measurements at times t_i and t_f are eigenvalues of H and $\tilde{H}$

satisfying $H|\phi_n\rangle = E_n|\phi_n\rangle$ and $\tilde{H}|\tilde{\phi}_m\rangle = \tilde{E}_m|\tilde{\phi}_m\rangle$. In every instance work is defined as $w = \tilde{E}_m - E_n$, which is distributed with probability

$$P(w) = \sum_{n,m} p_n p_{m,n} \delta(w - (\tilde{E}_m - E_n)), \qquad (1)$$

where $p_n = \langle\phi_n|\rho(t_0)|\phi_n\rangle$ is the probability to obtain the energy E_n and $p_{m,n} = |\langle\tilde{\phi}_m|U_{f,i}|\phi_n\rangle|^2$ is the transition probability between energy eigenstates when the system is driven by the evolution operator $U_{f,i} = U(t_f, t_0)$. From Eq. (1), we can derive the identity $\int dwP(w)\exp(-\beta w) = \sum_{n,m} p_n p_{m,n} \exp(-\beta(\tilde{E}_m - E_n))$. For a thermal initial state, $\rho(t_0) = \exp(-\beta H)/Z_0$, the remarkable identity derived first in Refs. [4,7] follows: $\langle\exp(-\beta w)\rangle = \tilde{Z}/Z = \exp(-\beta\Delta F)$, where F is the Helmholtz free energy.

Work measurement as a generalized measurement.—We can rewrite Eq. (1) as $P(w) = \mathrm{Tr}[\rho W(w)]$ where

$$W(w) = \sum_{n,m} p_{m,n} \delta(w - E_{m,n})|\phi_n\rangle\langle\phi_n|, \qquad (2)$$

with $E_{m,n} \equiv (\tilde{E}_m - E_n)$. Operators $W(w)$ define a positive operator valued measure as they form a set of non-negative operators which decompose the identity as $\int dwW(w) = I$. The operators $W(w)$ are not orthogonal since the number of values that w can take is larger than the dimension of the Hilbert space. A POVM defines the most general type of quantum measurement one can perform. Neumark's theorem [5] establishes that any POVM can be realized as a projective measurement on an enlarged system. Applying this observation for the case of work measurement, we conclude that it is always possible to design an apparatus such that (i) it produces an output w with probability $P(w)$, and (ii) when w is recorded, the system is prepared in a state ρ_w (that depends on ρ, w, and on the measurement implementation). There is not a unique method to implement a given POVM. Here, we present a simple strategy that can be used to evaluate work. For this purpose, we can couple the system $\mathcal{S}$ with an auxiliary system $\mathcal{A}$ in such a way that $\mathcal{A}$ gets entangled with $\mathcal{S}$ keeping a coherent record of the energy at two times. To do this, $\mathcal{S}$ and $\mathcal{A}$ must interact twice through an entangling interaction described by the Hamiltonian $H_I = \lambda H \otimes \hat{p}$, where λ is a constant and $\hat{p}$ is the generator of translations between the states $|w\rangle$ of $\mathcal{A}$. In the simplest case we can consider $\mathcal{A}$ with a continuous degree of freedom, where $\{|w\rangle, w \in \mathcal{R}\}$ is a basis of its space of states. The evolution operator $U_I = \exp(-iH_I t)$ is such that

$$U_I(|\phi_n\rangle \otimes |w = 0\rangle) = |\phi_n\rangle \otimes |w = E_n\rangle, \qquad (3)$$

with $t = 1/\lambda$ in appropriate units. Then, we drive the system with the operator $U_E = U_{f,i} = U(t_f, t_i)$. Finally, a new entangling interaction is applied. In summary, we apply the unitary sequence $U_{IEI} = \tilde{U}_I U_E U_I^\dagger$ [with $\tilde{U}_I = \exp(-i\lambda\tilde{H} \otimes \hat{p}t)$]. The resulting evolution transforms the initial product state $|\Psi(t_0)\rangle = |\phi_0\rangle \otimes |w=0\rangle$ into the final entangled state

$$|\Psi_f\rangle = \sum_{n,m} \langle\tilde{\phi}_m|U_E|\phi_n\rangle\langle\phi_n|\phi_0\rangle|\tilde{\phi}_m\rangle \otimes |w = E_{m,n}\rangle. \qquad (4)$$

At this stage we measure $\mathcal{A}$. The probability to find $\mathcal{A}$ in the state $|w\rangle$ is $P(w) = \langle\Psi_f|(I \otimes |w\rangle\langle w|)|\Psi_f\rangle$. It is simple to show that $P(w)$ is precisely the distribution given in Eq. (1). The state after detecting work w is $\rho_w = A_w \rho A_w^\dagger / P(w)$. Here, A_w is such that $W(w) = A_w^\dagger A_w$, $P(w) = \mathrm{Tr}(\rho W(w))$ and is given as

$$A_w = \sum_{n,m} \delta(w - E_{m,n})\langle\tilde{\phi}_m|U_E|\phi_n\rangle|\tilde{\phi}_m\rangle\langle\phi_n|. \qquad (5)$$

Noticeably, contrary to what happens in the standard two-time measurement scheme, the final state ρ_w is *not* an eigenstate of the final Hamiltonian.

Thus, we described a method to measure work, which is such that the outcome w is generated with probability $P(w)$, preparing the system in one of the nonorthogonal states ρ_w. In fact, although work is not a Hermitian operator, it can be measured with an ordinary POVM.

It is interesting to notice that the sequence of operations $U_{IEI} = \tilde{U}_I U_E U_I^\dagger$ has been realized in a recent experiment. The interaction U_I is precisely the one realized in a Stern Gerlach (SG) apparatus when the spin ($\mathcal{S}$) degrees of freedom interact with the motional ($\mathcal{A}$) degrees of freedom of a particle when it enters an inhomogeneous magnetic field. Then, the momentum of the particle is shifted by an amount that depends on the projection of the spin along the field. The magnitude of the shift depends on the field gradient and on the interaction time (controlled by the velocity of the particle). To realize U_{IEI} we need a sequence of two SG apparatuses with a spin driving field in between. Notably, this was done in a recent experiment [23] where SG type interactions were used to create coherent superpositions of momentum wave packets of an atomic beam. This remarkable experiment was done using an atom chip manipulating a falling cloud of ^{87}Rb atoms obtained from a BEC. The SG interaction U_I was implemented using a gradient pulse generated by coils in the chip. The gradient acts as a beam splitter and, as a consequence the atomic cloud splits into two pieces that move with different momenta, depending on their internal (Zeeman) state. As demonstrated in the experiment [23], the atoms behave as two-level systems and, after splitting the atomic cloud, the coils in the chip can generate radio frequency pulses coherently driving transitions between the Zeeman sublevels $|F, m_F\rangle = |2, 2\rangle$ and $|2, 1\rangle$. This implements the operator U_E, the second step of the U_{IEI} sequence. Finally, as shown in Ref. [23], a new U_I interaction can be applied to split the wave packet for a second time. As a result, four atomic clouds are produced, whose densities were measured by recording the shadow of the atoms in a resonant absorption experiment, tuned to an appropriate transition.

Here, we simply stress that a recent experiment performed with a different purpose [23], can be interpreted as realization of the work measurement method presented above. In that case, the initial and final Hamiltonians are defined by the gradient pulses (and are proportional to the interaction times) while the driving field is determined by the intermediate radio frequency pulses. Each of the four spots observed in the final image correspond to one of the four results of the POVM. Thus, the image in Ref. [23] directly reveals the work distribution for a single driven spin-1/2 particle. Different driving processes can be easily implemented.

Work estimation through phase estimation.—The above method to measure work naturally translates into a quantum algorithm that efficiently samples $P(w)$. The algorithm would run on a quantum computer which could be used to efficiently estimate moments of the work distribution. The method is a variant of the phase estimation algorithm [6], that plays a central role in many quantum algorithms. We consider an N-qubit system $\mathcal{S}$ ($D_{\mathcal{S}} = 2^N$) and an M-qubit ancilla $\mathcal{A}$ ($D = 2^M$ determines the precision of the sampling, as described below). We assume for simplicity that the Hamiltonians H and $\tilde{H}$ have bounded spectra that take values between $\pm E_M/2$ (this condition can be relaxed).

The algorithm below produces an m-bit string output x with a probability $P_D(x)$, which is a coarse-grained version of the work distribution $P(w)$ given in (1). Each integer x identifies a certain amount of work through the identity $w = 4E_M x/D$. Positive (negative) values of w correspond to $0 < x \leq D/4$ ($3D/4 \leq x \leq D-1$). The quantum algorithm for sampling $P(w)$, shown in Fig. 1, has six steps: (i) prepare the initial state $|x=0\rangle$ for $\mathcal{A}$ and ρ for $\mathcal{S}$; (ii) apply a quantum Fourier transform (QFT) on $\mathcal{A}$ mapping $|x\rangle$ onto its conjugate state $|\tilde{x}\rangle = U_{\mathrm{QFT}}|x\rangle = 1/\sqrt{D}\sum_{t=0}^{D-1} e^{i(2\pi x t/D)}|t\rangle$; (iii) apply the controlled operator $U_I = \sum_{t=0}^{D-1} |t\rangle\langle t| \otimes U^{\dagger t}$, where $U^t = \exp(-i\pi H t/4E_M)$; (iv) apply the unitary driving U_E over $\mathcal{S}$; (v) apply another controlled operation $\tilde{U}_I = \sum_{t=0}^{D-1} |t\rangle\langle t| \otimes \tilde{U}^t$, with $\tilde{U} = \exp(-i\pi\tilde{H}t/4E_M)$; (vi) apply the inverse QFT in $\mathcal{A}$ and measure its state in the $|x\rangle$ basis. The algorithm applies

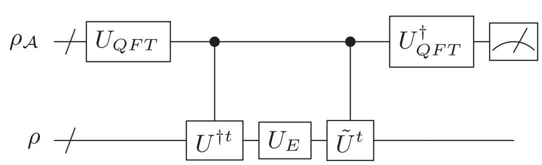

FIG. 1. Quantum circuit for the estimation of work probability distribution. The initial state of the auxiliary M-qubit system is a pure state $\rho_{\mathcal{A}} = |\psi_{\mathcal{A}}\rangle\langle\psi_{\mathcal{A}}|$ with $|\psi_{\mathcal{A}}\rangle = |x=0\rangle$. When the initial state of the system is pure given by $|\phi\rangle = \sum_{n=1}^{D_{\mathcal{S}}} c_n|\phi_n\rangle$ then the state of $\mathcal{S}$ and $\mathcal{A}$ just before the measurement is $|\Psi\rangle_{\mathcal{S},\mathcal{A}} = \frac{1}{D}\sum_{n,m=1}^{D_{\mathcal{S}}} c_n\langle\tilde{\phi}_m|U_E|\phi_n\rangle\sum_{t,x} e^{i(2\pi/D)t(x-(E_{m,n}/4E_M)D)}|w\rangle \otimes |\tilde{\phi}_m\rangle$.

the IEI sequence described above since the phase estimation subroutine is nothing but a standard measurement interaction.

The probability to detect x in $\mathcal{A}$ is $P_D(x) = \sum_{m,n} p_n p_{m,n} |F_D(4E_M(x/D) - E_{m,n})|^2$ where

$$|F_D(z)|^2 = \left|\frac{1}{D}\sum_{t=0}^{D-1} e^{-i(\pi z/2E_M)t}\right|^2 = \frac{1}{D^2}\frac{\sin^2(\frac{\pi z D}{4E_M})}{\sin^2(\frac{\pi z}{4E_M})}. \tag{6}$$

The distribution $P_D(x)$ is a coarse-grained version of the true work distribution $P(w)$ given in Eq. (1). Thus, $P_D(x)$ is the convolution between $P(w)$ and the filter function defined in Eq. (6):

$$P_D(x) = \int dw' \left|F_D\left(4E_M\frac{x}{D} - w'\right)\right|^2 P(w'). \tag{7}$$

The operators $A_D(x)$ defining the POVM are such that $P_D(x) = \mathrm{Tr}(\rho A_D^\dagger(x) A_D(x))$. They are also a convolution between the exact expression Eq. (5) and a filter function, i.e., $A_D(x) = \int dw' F_D(4E_M(x/D) - w')A(w')$.

It is simple to show that $P_D(x)$ rapidly approaches $P_{cg}(x)$, defined as the convolution of $P(w)$ with a rectangular function (which is unity for $|w| \leq 2E_M/D$ and zero otherwise). In fact, if $P(w)$ is bounded, then it is straightforward to show that $||P_{cg} - P_D||_\infty = \mathcal{O}(||P||_\infty/D)$. Therefore, the difference between $P_D(x)$ and $P_{cg}(x)$ decreases exponentially with the size of $\mathcal{A}$. In Fig. 2 we compare $P_{cg}(w)$ and $P_D(w)$ in a quenched process between two random Hamiltonians H and $\tilde{H}$. As $N = 10$, the number of different values of w is 2^{20}. It is clear that even for a small $\mathcal{A}$ (with $M = 5$ qubits), the sampling of the coarse-grained work distribution is highly accurate.

Estimating the free energy by sampling over the work distribution.—Sampling the work distribution $P(w)$ can be useful to efficiently estimate its moments. In turn, using Jarzynski identity, this can enable the estimation of the free energy of quantum states. For this one needs the expectation $\int dw P(w)\exp(-\beta w)$. The above quantum algorithm enables sampling the coarse-grained distribution $P_D(x)$, that can be used to efficiently estimate averages such as $\langle w\rangle$ with an accuracy that depends on the number of sampling points, K, as $1/\sqrt{K}$. So, for fixed precision (independent of the dimensionality of the Hilbert space of $\mathcal{S}$) this method is efficient. In Fig. 2 we show the dependence of the estimated ΔF with the number of times the distribution $P_D(x)$ is sampled (for two random Hamiltonians of a system of $N = 10$ qubits). However, as it is the case for classical systems, this strategy is not always efficient. In fact, efficiency depends on the properties of $P(w)$, because negative values of work, for which $\exp(-\beta w)$ is large are typically underrepresented in the sampling process (a situation that becomes worse at low temperatures).

Summary and comparison with previous work.—We showed that work measurement is a generalized quantum

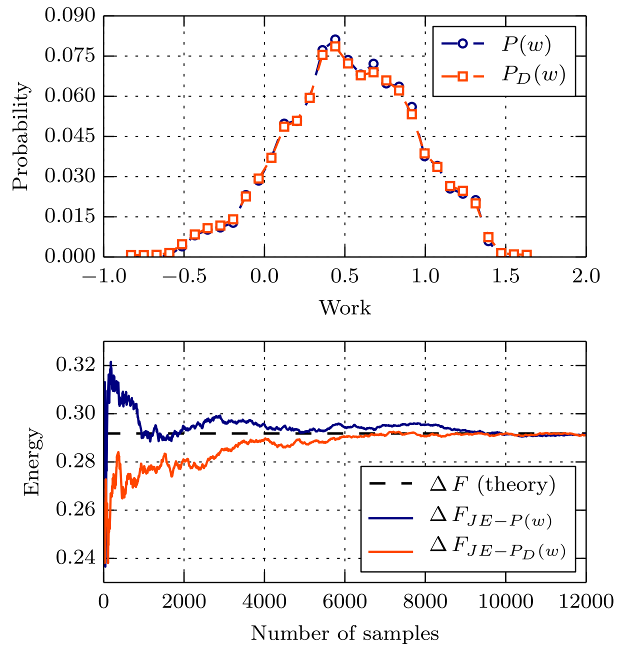

FIG. 2 (color online). Top: Comparison of the coarse-grained version of the exact probability distribution [given by Eq. (1)] with the probability distribution generated by the algorithm [Eq. (7)]. For this example a system $\mathcal{S}$ of 10 qubits was used (therefore giving 2^{20} different possible values of work), while the ancilla $\mathcal{A}$ was composed of only 5 qubits. Bottom: Free energy estimation using Jarzynski's equality and work values sampled from the exact distribution, $P(w)$, and the distribution resulting from the algorithm, $P_D(w)$. The exact value of the free energy difference is also shown, calculated as the ratio of the partition functions.

measurement (a POVM). This observation inspired a new method to measure work by performing a projective measurement on an enlarged system at a single time. This method inspires a new interpretation of an existing double SG experiment [23] and also a new quantum algorithm to efficiently sample a coarse-grained version of the work distribution $P(w)$. This algorithm could run in a quantum computer producing an M-bit output x with a probability $P_D(x)$, which is such that $P_D(x) = P(w \in I_x)$ with an accuracy that grows exponentially with M. Here, $w \in I_x$ iff $|w \mp 4E_M x/D| \leq 2E_M/D$ (where the $\mp$ sign respectively corresponds to the cases $0 \leq x \leq D/4$ and $3D/4 \leq x \leq D-1$). It is worth comparing this new method with the evaluation of the characteristic function of $P(w)$ ($\chi(s)$) [14,15]. In that case, the estimation of the expectation value of a single qubit operator is required for each value of s. By doing this, one can efficiently estimate work averages, which are obtained from derivatives of $\chi(s)$ at the origin. However, this method is not efficient to sample $P(w)$, which is obtained as the Fourier transform $\chi(s)$: To achieve the same precision we attain using M qubits in $\mathcal{A}$, the Ramsey method [14,15] would need to evaluate $\chi(s)$ in 2^M points. Our method allows the efficient estimation of global properties of $P(w)$ (like periodicities) and of the free energy for certain families of Hamiltonians.

Finally, we stress that in order to evaluate free energies, our method requires a thermal equilibrium state $\rho = \exp(-\beta H)/Z_\beta$ as a resource (the same as in [14,15]). However, this resource is not necessary if we use the recently proposed quantum Metropolis algorithm that enables the efficient sampling over the Gibbs ensemble [24].

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