Work statistics of charged noninteracting fermions in slowly changing magnetic fields

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We consider N fermionic particles in a harmonic trap initially prepared in a thermal equilibrium state at temperature β^{-1} and examine the probability density function (pdf) of the work done by a magnetic field slowly varying in time. The behavior of the pdf crucially depends on the number of particles N but also on the temperature. At high temperatures ($\beta \ll 1$) the pdf is given by an asymmetric Laplace distribution for a single particle, and for many particles it approaches a Gaussian distribution with variance proportional to N/β^2. At low temperatures the pdf becomes strongly peaked at the center with a variance that still linearly increases with N but exponentially decreases with the temperature. We point out the consequences of these findings for the experimental confirmation of the Jarzynski equality such as the low probability issue at high temperatures and its solution at low temperatures, together with a discussion of the crossover behavior between the two temperature regimes.

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I. INTRODUCTION

Fluctuation theorems that allow us to extract thermal equilibrium properties out of nonequilibrium processes, such as the Jarzynski equality (JE) [1]

$$\langle e^{-\beta w} \rangle = e^{-\beta \Delta F}, \quad (1)$$

have attracted considerable attention recently. Here w is the work performed by a time-dependent force acting on a system initially prepared in a thermal equilibrium at inverse temperature β; the average denoted by angular brackets $\langle \cdots \rangle$ is sufficiently taken over many realizations of the nonequilibrium work w obtained by repeated experiments with the same initial condition and force protocol. This fascinating equality was used for measuring the free-energy difference achieved in folding and unfolding processes of RNA [2]. A series of experiments followed and confirmed the JE for a macrosopic mechanical oscillator [3] and a colloidal particle [4]. Those experiments deal with a classical *single* particle. On the other hand, the generalization of Eq. (1) to quantum mechanical systems has been obtained in Refs. [5–10], see also the recent reviews [11,12].

The experimental confirmation of the JE crucially depends on the probability for observing the work that makes the most dominant contribution to the exponential average $\langle e^{-\beta w} \rangle = \int_{-\infty}^{\infty} e^{\Phi(w)}$, where $\Phi(w) = -\beta w + \ln P(w)$, with $P(w)$ being the probability density function (pdf) of the work. For concreteness, we assume that the pdf happens to be Gaussian as found, for example, in Ref. [3], but also in the presently studied case for many particles and at high temperatures: $P(w) = \exp[-(w - \langle w \rangle)^2/2\sigma^2]/\sqrt{2\pi\sigma^2}$ with $\sigma^2 = \langle w^2 \rangle - \langle w \rangle^2$ denoting the variance of work. Then the principal contribution to the exponential average is determined by the maximum of $\Phi(w)$, that is, by the condition $\partial\Phi(w)/\partial w|_{w=w_t} = 0$, yielding for the dominant work $w_t = \langle w \rangle - \beta\sigma^2$. The probability of the occurrence of this value then becomes $P(w_t) = e^{-\beta^{2\sigma^2/2}}/\sqrt{2\pi\sigma^2}$. This has a nontrivial consequence for experimental observations of work done on a many-particle system. Since the variance of the work σ^2 is related to an energy fluctuation, in a weakly or noninteracting system it increases proportionally to the number of particles N. This poses the difficulty of probing an improbable event. One may attempt to circumvent this problem by consulting the Crooks-Tasaki relation [6,9] that connects the work pdfs for forward and backward processes $p(w)$ and $p_B(w)$, respectively, by

$$\frac{p(w)}{p_B(-w)} = e^{\beta(w-\Delta F)}. \quad (2)$$

This relation may still give the free-energy difference in cases when the use of the JE is hampered by poor statistics. Since the free-energy difference coincides with the particular value of work at which the forward and backward pdfs $p(w)$ and $p_B(-w)$ agree with each other, the probability of observing this value $p(w = \Delta F)$, however, must be large enough to guarantee a reliable estimate of the free energy. It turns out that for a system of noninteracting fermions $p(w = \Delta)$ becomes exponentially small with the number N of fermions due to the extensivity of ΔF making it again difficult if not impossible to determine ΔF.

The purpose of this work is to illustrate the above discussion through a specific example and in addition, to suggest a way for observing work fluctuations in a many-particle system. For this purpose we consider N spinless electrons moving in a two-dimensional harmonic trap subject to a time-dependent magnetic field. We assume adiabatically slow changes of the field so that the eigenvalues of the instantaneous Hamiltonian do not cross during the force protocol. The restriction on the field strength imposed by this assumption is discussed. Furthermore, we employ the quantum generalization of the JE based on two-point measurements of energy [5,8], and focus on the temperature dependence of the resulting pdf. At high temperatures the pdf for a single particle follows an asymmetric Laplace distribution that yields null change in the free energy of the system. With increasing N, at a fixed temperature, the pdf widens and its value at w_t is indeed shown to be exponentially small for larger N. By contrast, lowering temperature makes the pdf extremely narrow and leads to appreciably larger values of $P(w_t)$ even for large N as long as the temperature is low as $\beta = c \ln N$ with c being a constant of the order of unity. We also point out the crossover between the low-temperature and the high-temperature behaviors.

II. CHARGED PARTICLE IN A MAGNETIC FIELD

We begin with the Hamiltonian for a single particle of mass m moving in a two-dimensional isotropic harmonic trap with curvature $m\omega_0^2$ in the presence of a uniform magnetic field $\mathbf{B} = B\hat{z}$:

$$\mathcal{H}_B = \frac{\Pi_x^2}{2m} + \frac{\Pi_y^2}{2m} + \frac{1}{2}m\omega_0^2(x^2 + y^2), \quad (3)$$

where the kinematic momenta Π_x and Π_y are given by

$$\Pi_x = p_x - (eB/2c)y, \quad \Pi_y = p_y + (eB/2c)x$$

with the symmetric gauge chosen for the vector potential $\mathbf{A} = (1/2)\mathbf{r} \times \mathbf{B}$. We neglect the spin of the particle and the respective Zeeman energy of the spin in the applied magnetic field. Since we do not take into account any spin-flip processes, spin-up and spin-down particles can be dealt with separately. The inclusion of spin would merely lead to a more cumbersome formulation, but leaves the main conclusions unaffected. Therefore, throughout our study we shall not consider the spin of the particles. Also note that for $\omega_0 = 0$, Eq. (3) yields the model Hamiltonian describing Landau diamagnetism. This phenomenon has been examined in many-electron systems. Hence, when particle statistics comes into question in the latter part of our work, we shall consider fermions with their spin degrees of freedom discarded. The oscillation frequency of the particle is then given by $\omega^2 \equiv \omega_0^2 + \omega_c^2/4$ with the cyclotron frequency $\omega_c = eB/mc$. The eigenstates $|n,\ell;B\rangle$ of the Hamiltonian are specified by a radial quantum number $n = 0,1,2,\ldots$ and an angular quantum number $\ell = 0, \pm 1, \pm 2, \ldots$. The corresponding energy eigenvalues satisfying

$$\mathcal{H}(B)|n,\ell;B\rangle = E_{n,\ell}(B)|n,\ell;B\rangle \quad (4)$$

are

$$E_{n,\ell}(B) = \hbar\omega(2n + 1 + |\ell|) + \tfrac{1}{2}\hbar\omega_c\ell\,. \quad (5)$$

These energy levels form parabolic branches as functions of the magnetic field B (see Fig. 1). At $B = 0$ they start out at $E_{n,l}(0) = \hbar\omega_0 m$ where $m = 2n + 1 + l = 1,2,\ldots$ with m-fold degeneracy. When $B \neq 0$, a state with, say positive ℓ, rotating anticlockwise is no longer degenerate with the corresponding clockwise rotating state with $-\ell$, giving rise to orbital magnetization. For a single particle system simple algebra leads to the exact form of the partition function

$$\mathcal{Z} = \sum_{n,\ell} e^{-\beta E_{n,\ell}} = [2\cosh(\tilde{\beta}\sqrt{1+\gamma^2}) - 2\cosh(\tilde{\beta}\gamma)]^{-1}, \quad (6)$$

where we introduced the dimensionless temperature $\tilde{\beta} \equiv \beta\hbar\omega_0$ and the frequency ratio $\gamma \equiv \omega_c/(2\omega_0) = eB/(2mc\omega_0)$.

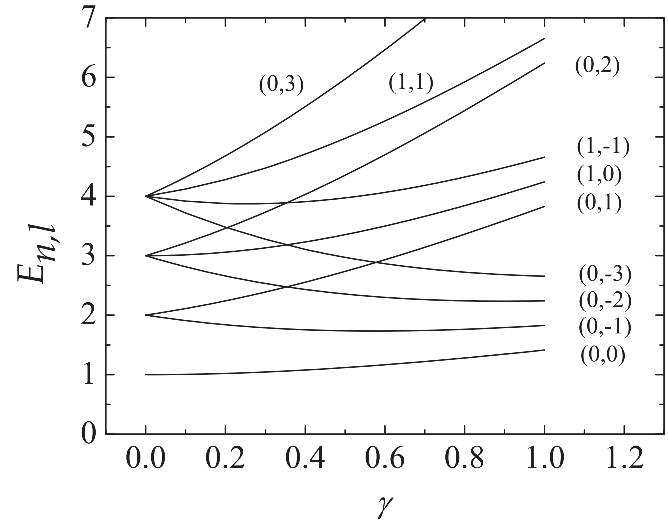

FIG. 1. Single-particle energy levels are displayed as functions of the field strength (γ). Only the lowest levels with $2n + |\ell| \leqslant 3$ are shown. The integer numbers at the right margin denote the quantum numbers (n,ℓ).

Hereafter we will drop the tilde for notational simplicity and use $\hbar\omega_0$ as an energy unit. At low temperatures and in the linear response regime ($\beta \gg 1$ and $\gamma \ll 1$) the partition function becomes $\mathcal{Z} \approx e^{-\beta}(1 - \beta\gamma^2/2)$. For the magnetic susceptibility $\chi = -\partial^2 F/\partial B^2$, wherein $F = -\beta \ln \mathcal{Z}$ denotes the free energy, one finds that in this limit χ is a negative constant, indicating the presence of orbital diamagnetism. On the other hand, at high temperature ($\beta \gg 1$) we obtain $\mathcal{Z} \approx 1/\beta^2$ which is the partition function of a classical particle moving in a two-dimensional harmonic potential. In accordance with van Leeuwen's theorem the classical partition function is independent of the magnetic field. This indicates that a free-energy change due to a uniform magnetic field is appreciable only at low temperatures. In the context of the Jarzynski equality (JE) this is equivalent to the statement that the work done by applying the fields should follow a probability density function (pdf) that yields $\langle e^{-\beta w}\rangle = 1$ at high and $\langle e^{-\beta w}\rangle \neq 1$ at low temperatures.

III. WORK CHARACTERISTIC FUNCTION FOR SINGLE PARTICLE

The work done by slowly switching on a magnetic field is determined by two measurements of the energy, one at time $t = 0$ when the field $B(0) = 0$ starts to grow, and the second one at time τ when the field has reached its final value $B(\tau) = B$ at the end of this protocol. The work then is given by the difference of these two energies. Here we assume that the field changes in such a slow way that it does not induce transitions between the energy eigenvalues $E_{n,\ell}(t) \equiv E_{n,\ell}[B(t)]$ of the instantaneous Hamiltonian $\mathcal{H}(t) \equiv \mathcal{H}[B(t)]$. This requires that different branches of instantaneous eigenvalues do not cross each other during the protocol. A wave function initially prepared as $\psi(t_0) = \sum_{n,\ell} c_{n,\ell}|n,\ell;t_0\rangle$ then adiabatically changes to become $\psi(t) = \sum_{n,\ell} c_{n,\ell}|n,\ell;t\rangle$ where $|n,\ell;t\rangle \equiv |n,\ell;B(t)\rangle$ denotes the eigenvectors of the instantaneous Hamiltonian at time t. For the time-evolution operator $U(t,t_0)$ relating $\psi(t_0)$ to $\psi(t) = U(t,t_0)\psi(t_0)$ we then obtain the simple expression

$$U(t,t_0) = \sum_{n,\ell} |n,\ell;t\rangle\langle n,\ell;t_0|. \qquad (7)$$

The work statistics can be determined by evaluating the characteristic function with the help of the relation [8,10]

$$G(u) = \int_{\infty}^{-\infty} dw e^{iuw} P(w) = \langle e^{iu\mathcal{H}_H(\tau)} e^{-iu\mathcal{H}_0}\rangle_{\rho_0} \qquad (8)$$

with the Hamiltonian in the Heisenberg picture $\mathcal{H}_H(\tau) = U^\dagger(\tau,0)\mathcal{H}(\tau)U(\tau,0)$, where $P(w)$ is the work pdf, and u denotes the variable conjugate to work. Here $\langle X\rangle_{\rho_0} = \mathrm{Tr}\, X\rho_0$ is the average of X with respect to the density matrix $\rho_0 = e^{-\beta\mathcal{H}(0)}/\mathcal{Z}_0$ describing the initial canonical state with the partition function $\mathcal{Z}_0 = \mathrm{Tr}\, e^{-\beta\mathcal{H}(0)}$.

Using Eq. (7) we find for the Hamiltonian $\mathcal{H}^H(\tau)$ the spectral representation

$$\mathcal{H}^H(\tau) = \sum_{n,\ell} E_{n,\ell}(\tau)|n,\ell;0\rangle\langle n,\ell;0| \qquad (9)$$

which happens to be diagonal with respect to the eigenbasis of $\mathcal{H}_0$. Hence for a single-particle system the characteristic function is given by

$$\begin{aligned} G(u) &= (1/\mathcal{Z}_0)\sum_{n,\ell} e^{iu\Delta_{n,\ell}} e^{-\beta E_{n,\ell}(0)} \\ &= (1/\mathcal{Z}_0)[2\cosh(\beta - iu\Delta_{0,0}) - 2\cos(u\gamma)]^{-1}, \end{aligned} \qquad (10)$$

where

$$\Delta_{n,\ell} = E_{n,\ell}(B) - E_{n,\ell}(0) \qquad (11)$$

denotes the work performed along the adiabatic branch indexed by n,ℓ. Here the partition function $\mathcal{Z}_0$ is given by Eq. (6) with $\gamma = 0$.

Since for the approximate form of the characteristic function [Eq. (10)] to hold, energy levels must not cross, one has to restrict the maximally reached field strength such that those levels that initially are populated do not cross when the field is slowly ramped up. For an initially populated set of energy values the critical value of the field parameter γ_c is given by the minimum value of γ for which a pair of levels crosses, that is, if $E_{n,\ell} = E_{n',\ell'}$. Here only those quantum numbers (n,l) and (n',l') contribute that are initially populated. This gives an equation for γ_c as $1/\gamma_c^2 = [\delta\ell/\delta\bar{n}]_m^2 - 1$, where $\bar{n} = 2n + |\ell|$, $\delta\bar{n} = \bar{n} - \bar{n}'$, $\delta\ell = \ell - \ell'$, and $[X]_m$ denotes the maximum value of X. One then finds for γ_c the relation

$$\sqrt{\gamma_c^2 + 1}/\gamma_c = 2[\bar{n}]_{\max} + 1 = 2E_{\bar{n}_m}(0) - 1. \qquad (12)$$

Since the initial energy states are weighed by $\bar{n}e^{-\beta E_{\bar{n}}(0)}$, Eq. (10) is approximately correct if $\beta E_{\bar{n}_m}(0) \gtrsim 1$, which together with Eq. (12) gives the upper limit of the field strength ensuring the validity of Eq. (10):

$$\gamma < \beta/(2\sqrt{1-\beta}). \qquad (13)$$

When $\beta > 1$ the ground state makes the dominant contribution to Eq. (10) and it does not cross any other level, as indicated by the above criterion. For higher temperatures γ has to remain sufficiently small and therefore $\beta\gamma \ll 1$. Finally we note that when $\gamma \simeq \gamma_c$, 2γ corresponds to the maximum level spacing between adjacent energy states. This implies that the level discreteness cannot be resolved when the condition $\beta\gamma \ll 1$ is met. It is therefore anticipated that Eq. (10) should coincide with the characteristic function obtained in the classical limit, that is, by neglecting the energy level discreteness.

IV. CLASSICAL CHARACTERISTIC FUNCTION AND WORK PDF

A. Single particle

Next we evaluate the characteristic function describing the statistics of work applied to a classical charged particle by a slowly increasing magnetic field. For a general protocol defining a time-dependent Hamiltonian function $H(\mathbf{z},t)$ the characteristic function is given by the phase space integral [1]

$$G_c(u) = \int d\mathbf{z} e^{iu\{H[\mathbf{Z}(\mathbf{z},\tau),\tau] - H_0(\mathbf{z})\}} e^{-\beta H(\mathbf{z},0)}/\mathcal{Z}_0^c, \qquad (14)$$

where $\mathcal{Z}_0^c = \int d\mathbf{z} \exp[-\beta H(\mathbf{z},0)]$ denotes the classical partition function of the field-free system at inverse temperature β,$\mathbf{z}$ are canonical phase space coordinates, and $\mathbf{Z}(\mathbf{z},t)$ denotes the phase space point reached at time t from the initial point $\mathbf{z}$ according to the time evolution governed by $H(\mathbf{z},t)$. For an adiabatic change of the magnetic field the instantaneous system energy $E[B(t)] = H[\mathbf{Z}(\mathbf{z},t),t]$ can be expressed in terms of conserved action variables $J_\rho = \oint d\rho p_\rho$ and $J_\phi = \oint d\phi p_\phi$, where (ρ,ϕ) are polar coordinates of the particle position with $\rho = 0$ at the minimum of the harmonic potential. The corresponding canonical momenta are (p_ρ, p_ϕ). In the present case p_ϕ is conserved when we find $J_\phi = 2\pi p_\phi$. For the other action one obtains after some algebra $J_\rho = -|J_\phi|/2 + \omega_c J_\phi/(2\omega) + \pi E(B)/\omega$. In passing we note that the quantization conditions of the actions $J_\rho = 2\pi n\hbar$ and $J_\phi = 2\pi\ell$ lead to the energy eigenvalues as given by Eq. (5). This is to be expected since in Eq. (5) the zero-point energy was neglected. The expression for J_ρ can be solved for the energy to yield

$$E(B) = (\omega/\pi)(J_\rho + J_\phi/2) - \omega_c J_\phi/(4\pi). \qquad (15)$$

The phase space integral of the characteristic function (14) can then be written in terms of action and angle variable becoming

$$\begin{aligned} G_c(u) &= \mathcal{Z}_0^{-1}(2\pi)^2 \int dJ_\rho dJ_\phi e^{iu[E(B)-E(0)]} e^{-\beta E(0)} \\ &= \{[1 - i(u/\beta)(\sqrt{1+\gamma^2} - 1)]^2 + (\gamma u/\beta)^2\}^{-1}, \end{aligned} \qquad (16)$$

where in the first line the integration over the angle variables was performed resulting in the factor of $(2\pi)^2$. The above classical characteristic function can as well be obtained in the small β limit of Eq. (10). Here we note that in the high-temperature limit small values of u mainly determine the behavior of the pdf and hence one cannot simply let $\beta \to 0$. A way to take into account this subtlety is to introduce u/β as a variable kept independent of the limiting process.

The inverse Fourier transform of $G_c(u)$ then gives the classical pdf of work

$$P_c(w) = \frac{\beta\alpha_+\alpha_-}{\alpha_- - \alpha_+}[\Theta(w)e^{\alpha_-\beta w} + \Theta(-w)e^{\alpha_+\beta w}] \qquad (17)$$

with $\alpha_\pm = [(1-\sqrt{1+\gamma^2}) \pm \gamma]^{-1}$ and $\Theta(x) = 1$ for $x > 0$, and $\Theta(x) = 0$, otherwise. The work pdf is given by an asymmetric Laplace distribution, with average

$$\langle w \rangle_1 = 2(\sqrt{1+\gamma^2} - 1)/\beta \tag{18}$$

and variance

$$\sigma_1^2 = 4\sqrt{1+\gamma^2}(\sqrt{1+\gamma^2} - 1)/\beta^2. \tag{19}$$

This implies a relation between the average and variance of the work given by

$$\beta\Gamma = \frac{2\langle w \rangle_1}{\sigma_1^2} \tag{20}$$

with $\Gamma = 1/\sqrt{1+\gamma^2}$.

The validity of the Jarzynski equation $\langle e^{-\beta w} \rangle = 1$ follows both from Eq. (16) by putting $u = i\beta$ or likewise from Eq. (17) by performing the average exponential work.

B. N particles

For an N-particle system at high temperatures both the level discreteness and the particle statistics, that is, whether they are fermions or bosons, can be discarded. The N-particle characteristic function is then given by $G^{(N)}(u) \approx [G(u)]^N$. This leads to the following pdf of collective work done on N particles:

$$\begin{aligned} P_c^{(N)}(w) &= (2\pi)^{-1} \int dw e^{iuw + N \ln G_\tau(u)} \\ &\approx \frac{1}{\sqrt{2\pi N \sigma_1^2}} \exp\left[\frac{(w - N\langle w \rangle_1)^2}{2N\sigma_1^2}\right], \quad N \gg 1. \end{aligned} \tag{21}$$

The first line guarantees the extensive property of the free energy such that the Jarzynski equality holds, that is, $\int dw P_c^{(N)}(w) e^{-\beta w} = e^{-N\beta\Delta F}$ with ΔF being the free-energy changes for a single particle. In obtaining the second line we performed a steepest decent approximation of the integrand for large N and small u with finite u/N. Note that the resulting Gaussian approximation in general no longer conforms with the Jarzynski equality since the tail of the pdf that dominates the average of exponential work is not properly approximated by a Gaussian which only represents the central part of the work pdf. This issue was also observed in Ref. [13] in a molecular dynamics simulation of a Joule heating experiment [13]. In the limit of weak magnetic fields the average work and its variance become

$$\langle w \rangle \approx N\gamma^2/\beta, \quad N \gg 1, \quad \gamma \ll 1 \tag{22}$$

and

$$\sigma_N^2 \approx 2N\gamma^2/\beta^2, \quad N \gg 1, \quad \gamma \ll 1, \tag{23}$$

where terms of the order of γ^4 are neglected. With this approximation the Jarzynski equality is recovered in the Gaussian approximation.

Numerically exact results of $P_c^{(N)}(w)$ are presented for various values of N in Fig. 2. As N increases the pdf shifts toward larger positive work values, and broadens at the same time. This behavior can also be seen from the analytic approximate expression of the pdf for $N \gg 1$ in the second line of Eq. (21). Both the average work and the variance of the work increase linearly with the particle number N.

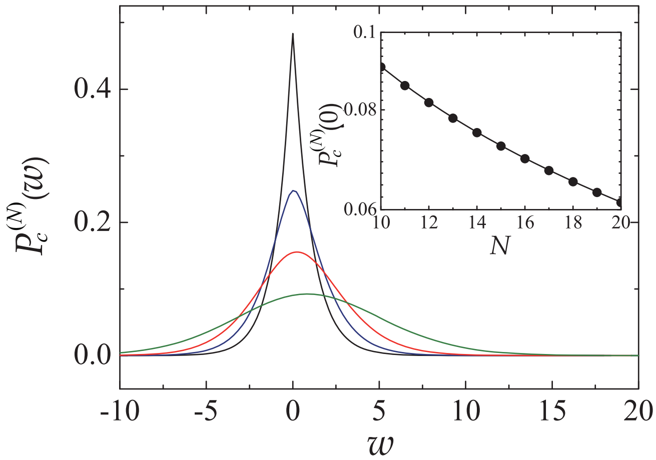

FIG. 2. (Color online) Classical work pdfs $P_c^{(N)}(w)$ as a function of work at fixed field strength $\gamma = 0.1$ and $\beta = 0.1$ for $N = 1, 2, 4, 10$ in the order of decreasing peak height. The inset shows the exponential decay of $P_c^{(N)}(0)$ with N.

We now examine the probability for observing the work w_t that dominates the average exponential work in the Jarzynski equality. As explained above it is given by the location of the maximum of the integrand $\exp(-\beta w) P_c^{(N)}(w)$ with respect to w. Using for large N and small fields the Gaussian approximation of the work pdf as given by the second line of Eq. (21) together with Eqs. (18) and (19), one obtains the dominant work as given by the negative average work $w_t = -\langle w \rangle = -N\gamma^2/\beta$. The probability density at this value becomes with $P_c^{(N)}(w_t) \propto \exp(-N\gamma^2)$ exponentially small in N and eventually prohibitively small to verify the Jarzynski equality. This low probability issue also cannot be resolved by using the Crooks-Tasaki relation [6]. For the present classical case, in which the free energy remains unchanged by the presence of a magnetic field, the pdfs of the forward and the backward processes coincide with each other at $w = 0$ according to Eq. (2). Whether it is possible to reliably recover this value from a finite set of work data of a real or numerical experiment is determined by the value of the work pdf at $w = 0$ which can be exactly evaluated from Eqs. (21) and (16) yielding

$$P_c^{(N)}(w=0) = \frac{\beta|\alpha_+\alpha_-|^N}{(\alpha_+ - \alpha_-)^{2N-1}} \frac{(2N-2)!}{(N-1)!(N-1)!} \tag{24}$$

which for $N \gg 1$ becomes $P_c^{(N)}(w=0) \sim \beta e^{-N\gamma^2/4}$, again exponentially small. To avoid this probability catastrophe in dealing with many particles, the field strength may be tuned weak enough ($\gamma^2 N \ll 1$). Alternatively one may go to low temperatures where quantum effects lead to different scenarios. Rather than pursuing the first approach restricted to $\Delta F \approx 0$, we examine the low-temperature regime where the free-energy changes as a result of a magnetic field variation.

V. WORK STATISTICS AT LOW TEMPERATURES

A. Single particle

At low temperatures two factors matter: level discreteness and particle statistics. For a single particle the latter is still irrelevant. The characteristic function then is given by Eq. (10). Its inverse Fourier transform leads to the work pdf

$$P(w) = \sum_{n,\ell} \mathcal{W}_{n,\ell}\delta(w - \Delta_{n,\ell}), \quad (25)$$

where $\mathcal{W}_{n,\ell} = e^{-\beta E_{n,\ell}(0)}/\mathcal{Z}_0$ determines the weights of the peaks at $\Delta_{n,\ell}$ given in Eq. (10). In the high-temperature limit many levels contribute to yield a continuous form of the probability distribution. Note that for $\beta \ll 1$ the characteristic function Eq. (10) converges to the classical expression Eq. (16) and results in the work pdf given by Eq. (17). On the other hand, at low temperatures the work pdf of a single particle consists of a series of delta peaks and no longer displays the exponential tails of the asymmetric Laplace distribution valid at high temperatures. The largest weights at low temperatures are given by the ground state, and a few excited states, such as $(n,\ell) = (0,0)$, $(0,\pm 1)$, $(0,\pm 2)$, $(1,\pm 1)$, $(0,\pm 3)$ [note that the last two pairs have the same energy $E_{n,l}(0)$ and hence give the same weight]. These states actually contribute most to the free-energy change at low temperatures.

B. *N* fermions

Before discussing the many-particle case in more detail, we like to mention that the low-probability catastrophe is closely related to the particle number dependence of the width of the pdf. Figure 2 displays a broadening of the work pdf as N increases. As a quantitative indicator, we see that the average work and its variance for the classical N-particle system are N times larger than the respective quantities of the single-classical particle, meaning that Eq. (20) holds for any N. On the other hand, at low temperatures we will demonstrate that the variance of the pdf exponentially decays with temperature and Eq. (20) no longer holds.

For a quantum many-particle system we consider spinless charged noninteracting fermions that initially are in an equilibrium with a weakly interacting reservoir defining a chemical potential μ as well as a temperature $1/\beta$. Their initial density operator then reads $\rho_g = e^{-\beta[\mathcal{H}(0)-\mu\mathcal{N}]}/\mathcal{Q}_0$ with $\mathcal{Q}_0$ being the grand canonical partition function and $\mathcal{N}$ the operator that measures the total number of particles. The average particle number is determined through

$$N = \langle\mathcal{N}\rangle = \sum_{n,\ell} \frac{1}{1 + e^{\beta[E_{n,\ell}(0)-\mu]}}. \quad (26)$$

Under the assumption that the initial and final Hamiltonians conserve the particle number, that is, that $\mathcal{N}$ commutes with $\mathcal{H}_0$ and $\mathcal{H}(\tau)$, energies and particle numbers can be simultaneously measured both initially and finally. In general, during the protocol the particle number need not be conserved. The characteristic function for the statistics of the work and the particle exchange was found as [14]

$$\begin{aligned}\mathcal{G}(u,v) &= \sum_n \int dw e^{iuw+iv\Delta N} P(w,\Delta N)\\ &= \langle e^{iu\mathcal{H}_H(\tau)+iv\mathcal{N}_H(\tau)} e^{-iu\mathcal{H}(0)-iv\mathcal{N}(0)}\rangle_{\rho_g}, \quad (27)\end{aligned}$$

where $\langle X\rangle_{\rho_g} = \mathrm{Tr}\,\rho_g X$ and $P(w,\Delta N)$ denotes the joint pdf to find the work w and particle number change ΔN realized in an experiment with a specified protocol of duration τ. In analogy, to work the particle number exchange is given by the difference of the eigenvalues of the particle numbers in the final and the initial state.

Note that $\mathcal{G}(i\beta, -i\mu\beta) = \mathcal{Q}_\tau/\mathcal{Q}_0$ leading to a generalized Jarzynski equality for a grand canonical initial state. Equivalently,

$$\begin{aligned}\langle e^{-\beta w} e^{-\beta\mu\Delta N}\rangle &\equiv \sum_{n=-\infty}^{\infty} \int dw e^{-\beta w} e^{-\beta\mu\Delta N} \mathcal{P}(w,\Delta N)\\ &= e^{-\beta\Delta\Phi_G}, \quad (28)\end{aligned}$$

where the grand potential difference is defined as $\Delta\Phi_G = \Phi_G(\tau) - \Phi_G(0)$ with $-\beta\Phi_G = \ln\mathcal{Q}$. In the present case the number operator is a constant of motion, that is, $[\mathcal{H}(t),\mathcal{N}] = 0$ for all times during the protocol and therefore $\mathcal{N}_H(t) = \mathcal{N}(t) = \mathcal{N}(0)$. As a result, the characteristic function is constant with respect to v, that is, $G(u,v) = G(u,0) \equiv G(u)$ leading to $P(w,\Delta N) = P(w)\delta_{\Delta N,0}$. Putting $\mathcal{H}(\tau) = \mathcal{H}_B$ and $\mathcal{H}(0) = \mathcal{H}_0$, we can write the characteristic function as

$$\mathcal{G}(u) = \langle U^\dagger(\tau,0) e^{iu\mathcal{H}_B} U(\tau,0) e^{-iu\mathcal{H}_0}\rangle_{\rho_g}. \quad (29)$$

Adopting the occupation number representation as a usual approach to many particle systems we reach

$$\begin{aligned}\mathcal{G}(u) &= \langle e^{iu\sum_{n,\ell}\Delta_{n,\ell}N_{n,\ell}}\rangle_{\rho_g}\\ &= \prod_{n,\ell} (1 - \langle N_{n,\ell}\rangle + \langle N_{n,\ell}\rangle e^{iu\Delta_{n,\ell}}) \quad (30)\end{aligned}$$

for fermionic particles undergoing an adiabatic field switch. Here $N_{n,\ell}$ denotes the number of particles occupying the energy eigenstates defined by the quantum numbers n,ℓ. For fermionic particles $N_{n,\ell} = 0$ or 1. In obtaining the second equality we used the identity $N_{n,\ell}^2 = N_{n,\ell}$ and $e^{i\alpha N_{n,\ell}} = 1 - N_{n,\ell} + N_{n,\ell}e^{i\alpha}$. Also we discarded any level crossings as was done for the single-particle case. This imposes a limitation of the maximally reached field strength as a function of temperature and chemical potential requiring that

$$\gamma < \bar{\beta}/(2\sqrt{1-\bar{\beta}}). \quad (31)$$

This validity criterion for N particles can be obtained from the respective single-particle criterion by increasing the single-particle energy bound by the chemical potential such as $E_{\bar{n}_m} \approx \mu_F + \beta^{-1} \equiv \bar{\beta}^{-1}$, and replacing the true temperature β^{-1} by the effective energy scale $\bar{\beta}^{-1}$ in Eq. (13).

We numerically computed the characteristic function Eq. (30) and obtained the work pdf from its inverse Fourier transform, as given in the first line of Eq. (27). In Fig. 3(a) work pdfs at different temperatures are compared displaying the change from a smooth and broad distribution at $\beta = 1$ to a narrow one at $\beta = 10$; at intermediate temperatures shoulders indicated by arrows in the inset of Fig. 3(a) appear. At low temperatures the work pdfs strongly deviate from Gaussians. We further evaluated the average work and its variance. Most notably for different parameter values the average work divided by its zero-temperature limit w_0 collapses to a single curve depending solely on $N\gamma^2/(\beta w_0)$ [see panel (b) of Fig. 3]. The dependence of the average work at zero temperature w_0 on $N\gamma^2$ is displayed in the inset of Fig. 3(b) for two different values of N. This graph indicates that for small values of the field strength γ the parameter combination $N\gamma^2/(w_0\beta)$ essentially provides a measure of the temperature $1/\beta$. Accordingly the ratio $\langle w\rangle/w_0$ approaches unity for small values of $N\gamma^2/(w_0\beta)$. For large values of this parameter combination this ratio reaches the high-temperature asymptotics Eq. (22) displayed by the straight solid line in Fig. 3(b). The crossover between these two asymptotic regimes takes place in the region of $N\gamma^2/(w_0\beta) \approx 1$. It should be mentioned that not for all parameter values used in the plot the no-crossing condition (31) is satisfied. For example, those with $\gamma = 0.3$ and $N = 15$ violate this condition even at low temperatures. However, we confirmed that different parameter values can be chosen that yield the same value of $N\gamma^2/\beta$, conform with the condition Eq. (31), and render the same average work.

In order to visualize the deviations of the high-temperature behavior of the ratio of the work average and variance from its classical behavior Eq. (20) this ratio is displayed in Fig. 3(c) as a function of $\beta\Gamma = \beta/\sqrt{1+\gamma^2}$. At small values of $\beta\Gamma$ the work-variance ratio coincides with the classical result Eq. (20) represented by the solid straight line in Fig. 3(c) and starts to deviate from it for $\beta\Gamma \approx 3$. Most notably all data points for different parameter values still collapse onto a single curve. The increase of this ratio for small temperatures and hence large $\beta\Gamma$ values results from an exponential decay of the variance at decreasing temperatures [see the inset of Fig. 3(c)].

This indicates that at low temperatures the pdf is sharply centered at $\langle w\rangle$. As a rough approximation for the pdf we write $P_g(w) = \exp[-(w-\langle w\rangle)^2/2\sigma_N^2]/\sqrt{2\pi\sigma_N^2}$. Although the Gaussian form cannot reflect the fat tails as displayed in Fig. 3(a), it suffices for our discussion that concerns mainly the peak position and the variance. The probability for observing the dominant work is given by $P(w_t) = e^{-\beta\sigma^2 N/2}/\sqrt{2\pi\sigma_N^2}$. Note that for any noninteracting system σ_N^2 is an extensive quantity linearly increasing with the number of particles. This together with the temperature dependence of σ_N^2 leads to the conclusion that a crucial factor to determine $P(w_t)$ is the temperature; even for $N \gg 1$ the probability can still be appreciable if the temperature is low enough to make $\beta/\ln N \sim O(1)$. Temperatures to meet this criterion can be realized thanks to the logarithmic dependence of N, unlike the expectation from the high-temperature results where in order to obtain appreciable probability the temperature should be lowered as $\beta e^{-N\gamma^2} \sim O(1)$.

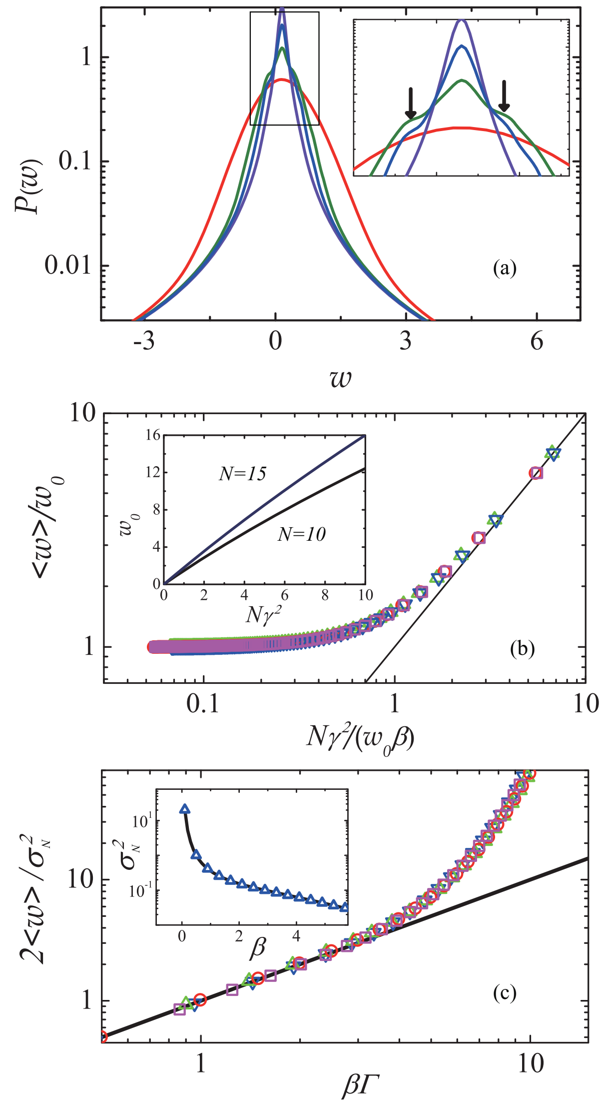

FIG. 3. (Color online) (a) Work pdfs for $N = 10$ and $\gamma = 0.1$ at $\beta = 1, 3, 5, 10$ in the peak height increasing order. The inset presents a blowup of the boxed area. (b) Low temperature deviation of the work average from its high-temperature value (the ordinate), where $\langle w_q\rangle = \langle w\rangle/w_0$ and $\beta_q = \beta w_0$ with w_0 denoting the work average at zero temperature. Data for systems with different particle numbers and field strength collapse onto a single curve. The different symbols indicate the cases with $N = 10$, $\gamma = 0.1$ ($\triangle$), $N = 15$, $\gamma = 0.1$ ($\circ$), $N = 10$, $\gamma = 0.3$ (∇), $N = 15$, $\gamma = 0.3$ ($\square$). (c) Crossover behavior of the ratio of average work and variance where the straight line corresponds to Eq. (20). Also here data for systems with different particle numbers and field strengths collapsing onto a single curve. The symbol code for different parameter values agrees with that of panel (b). The inset shows the temperature dependence of the variance for $N = 10$ and $\gamma = 0.1$. At low temperatures it exponentially decreases giving rise to the sharp increase of $\langle w\rangle/\sigma_N^2$.

VI. CONCLUSIONS

In summary we considered N fermionic particles moving in a harmonic trap and examined the statistics of the work done by a time-varying magnetic field. Our study was made under the assumption of an adiabatically slow protocol and restricted to magnetic fields of weak strength in order to avoid level crossings. In relation to the experimental confirmation of the Jarzynski equality for a many-particle system, we payed special attention to the probability for observing the dominant work $P(w_t)$ and its behavior depending on the temperature and the particle number. At high temperatures the width of the work pdf linearly grows with N/β^2, which leads to $P(w_t) \sim e^{-N\gamma^2}$ being exponentially small for large N. At low temperatures, on the other hand, the width of the pdf exponentially decreases with falling temperature, which makes $P(w_t)$ appreciable even for large N as long as $\beta \sim \ln N$.

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