Work fluctuations for Bose particles in grand canonical initial states

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We consider bosons in a harmonic trap and investigate the fluctuations of the work performed by an adiabatic change of the trap curvature. Depending on the reservoir conditions such as temperature and chemical potential that provide the initial equilibrium state, the exponentiated work average (EWA) defined in the context of the Crooks relation and the Jarzynski equality may diverge if the trap becomes wider. We investigate how the probability distribution function (PDF) of the work signals this divergence. It is shown that at low temperatures the PDF is highly asymmetric with a steep fall off at one side and an exponential tail at the other side. For high temperatures it is closer to a symmetric distribution approaching a Gaussian form. These properties of the work PDF are discussed in relation to the convergence of the EWA and to the existence of the hypothetical equilibrium state to which those thermodynamic potential changes refer that enter both the Crooks relation and the Jarzynski equality.

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I. INTRODUCTION

In recent years fluctuation theorems that allow to infer equilibrium properties of a system from nonequilibrium processes have attracted considerable attention. The Jarzynski equality (JE) \[1\] reading

\[
\langle e^{-\beta w} \rangle = e^{-\beta \Delta F},
\]

(1)

provides a prominent example of these relations. It relates the free energy change $\Delta F$ to the statistics of work $w$ that is performed by a time-dependent force acting on a system that initially is prepared in a canonical equilibrium state at the temperature $T = 1/k_B\beta$. The weight with which the average of the exponentiated work is performed is determined by the probability density function (PDF) of work, $p(w)$. It represents the frequency of outcomes from independent runs of the same force protocol starting in equilibrium at the same temperature. The free energy change $\Delta F$ gives the difference between free energies of the initial state and of a hypothetical thermal equilibrium state of the considered system at the initial temperature $T$ with clamped forces at the values at the end of the force protocol. First, the JE was found for classical systems and later on confirmed for quantum mechanical systems \[2,3\].

A similar form of the JE holds for grand canonical initial states (GCI) which allow both energy and particle number fluctuations. It then takes the form \[4,11\]:

\[
\langle e^{-\beta w} e^{\beta \mu n} \rangle_{\text{gc}} = e^{-\beta \Delta \Phi},
\]

(2)

where $w$ and $\beta$ are defined as above. Further, $\mu$ denotes the chemical potential of the reservoir, and $n$ the difference of the particle numbers at the end and at the beginning of the force protocol. Similarly as the work $w$ also the particle number change $n$ is a random quantity. These random outcomes are described by a joint PDF $p(w, n)$. Here $\Delta \Phi = \Phi_f - \Phi_i$ is given by the difference of the grand canonical potentials $\Phi_i$ and $\Phi_f$ which respectively correspond to the initial equilibrium state and to a hypothetical equilibrium state at the inverse temperature $\beta$ and chemical potential $\mu$ with clamped force values at the end of the force protocol.

While temperature is universally confined to positive values, the upper admissible bound of the chemical potential is system dependent. To illustrate this fact we consider a system of non-interacting identical particles for which the average particle number in a grand canonical potential at inverse temperature $\beta$ and chemical potential $\mu$ is determined by \[12\]

\[
N_{av} = \sum_n \frac{1}{e^{\beta (\epsilon_n - \mu)} + 1}, \tag{3}
\]

where the sum is performed over the single particle energy spectrum, and the $+$ and $-$ signs refer to Fermi-Dirac and Bose-Einstein statistics, respectively. Considering the case of a single particle spectrum which is bounded from below by the ground state, for fermions, the $+$ sign guarantees the convergence of the sum for any real value of the chemical potential. However, for a system made of bosons, this sum only converges if the chemical potential is smaller than the ground state energy. With the divergence of the average particle number the grand canonical partition function diverges and accordingly the grand canonical potential becomes neg-
ately divergent. In the context of the fluctuation theorem given by Eq. (2), this implies that the averaged exponentiated linear combination of work and number change, that is, the left hand side of Eq. (2), diverges for Bosonic systems under the action of protocols which lead to a lowering of the single particle ground state energy below the level of the chemical potential of the initial grand canonical equilibrium state.

The purpose of this work is to address this issue of the fluctuation theorem for GCI, Eq. (2). For a concrete discussion, we consider non-interacting bosons residing in a three-dimensional symmetric harmonic trap with equilibrium state. Section II is devoted to a brief introduction to the system. The single particle energy spectrum at time 0 is not specifically related to the condensation transition. The single particle energy spectrum at time 0 is given by

\[
\epsilon_\ell(t) = (\ell_x + \ell_y + \ell_z + 3/2)\hbar \omega(t)
\]

with a set of non-negative integers \( \ell \equiv (\ell_x, \ell_y, \ell_z) \).

A. Equilibrium properties

This many particle system is supposed to initially stay in equilibrium with a reservoir having prescribed values of the chemical potential \( \mu \) and the inverse temperature \( \beta \). For this initial equilibrium state the initial grand canonical partition function and the initial average number of particles are determined by

\[
Q_\ell = \prod_\ell \left[ 1 - ze^{\beta \epsilon_\ell(0)} \right]^{-1}
\]

\[
N_{av} = \sum_\ell \frac{1}{z^{-1}e^{\beta \epsilon_\ell(0)} - 1},
\]

where \( z = e^\beta \mu \) denotes the fugacity. The condensation fraction is given by \( N_0/N_{av} \) with \( N_0 \) denoting the particle occupancy in the ground state, \( N_0 = 1/(z^{-1}e^{\beta \epsilon_0(0)} - 1) \). For sufficiently large \( N_{av} \), the condensation curve falls onto the critical line, \( N_0/N_{av} = 1 - (T/T_c(0))^3 \) if \( T \leq T_c(0) \) and \( N_0/N_{av} = 0 \), otherwise, with the critical temperature \( T_c(0) = (N_{av}/\zeta(3))^{1/3}(\hbar \omega/k_B) \), where \( \zeta(3) \approx 1.202 \). When the number of particles is finite, the transition becomes smeared out and the critical temperature is modified as \( T_c = (1 - 0.7275N_{av}^{-1/3}) \).

In the sequel we shall use \( T_c \) as temperature unit.

B. Doing work

We here sketch a gedankenexperiment that elucidates the relevant steps implied by Eq. (2). Fig. 1(a) depicts the initial equilibrium state of the considered many particle system in weak contact with a reservoir that may exchange particles and energy with the system controlled by the chemical potential \( \mu \) and the inverse temperature \( \beta \). The grand potential \( \Phi_i = -k_B T \ln Q_\ell \) for this initial state is determined by the reservoir parameters as well as by the microscopic details such as the initial curvature of the potential defining the oscillation frequency \( \omega \). Once the system has approached the grand canonical equilibrium state, it is decoupled from the reservoir, its
energy and particle number are determined, and afterward the curvature of the trap is changed according to a designed protocol. Finally energy and particle number are again measured. The change of energy determines the work \( w \) performed on the system in this particular realization. The work and the particle number change \( n \) are finally registered. This procedure must be repeated many times, always starting from the same equilibrium state and following the same protocol such that the joint probability \( p(w, n) \) can be estimated, or, directly the exponential average \( \langle e^{-\beta (w-\mu n)} \rangle \) can be estimated. According to Eq. (2) this average value coincides with the ratio of the two partition functions. The denominator is given by the partition function of the initial system and hence determined by the initial initial trap curvature as well as by \( \beta \) and \( \mu \). The numerator refers to the hypothetical equilibrium of system with the final trap curvature see Fig. 1 (c).

There is no restriction for the finally reached trap curvature. In particular, the trap may be widened to such an extent that the ground state energy falls below the chemical potential of the initial state. Then the hypothetical equilibrium state is not properly defined and formally leads to a divergent grand canonical partition function and a negative, divergent grand canonical potential. At the same time the exponential average of \(-\beta (w-\mu n)\) also diverges.

### III. CHARACTERISTIC FUNCTION

Along with the JE, the Tasaki-Crooks relation \[^{2,19}\]^ reading

\[ e^{-\beta w} p(w) = e^{-\beta \Delta \Phi} p_0(-w), \]  

provides a connection between the PDFs \( p(w) \) of the original process and the PDF \( p_0(w) \) of the backward process for systems initially prepared in a canonical equilibrium state. Here the backward process starts at the hypothetical equilibrium state retracing the force protocol from its final to the initial value of the forward process. From the correspondence between Eq. (11) and Eq. (2), one may expect the existence of a Crooks-Tasaki relation for the GCI of the form

\[ e^{-\beta(w-\mu n)} p(w, n) = e^{-\beta \Delta \Phi} p_0(-w, -n). \]  

Integrating over \( w \) and summing over all possible values of \( n \), we indeed obtain the generalized form of JE for the GCI, as given in Eq. (2).

The proof of this relation may be obtained in an analogous way as for the canonical case \[^{2,3,8}\]^ based on the characteristic function \( G(u, v) \). It is given as the Fourier transform of the joint PDF \( p(w, n) \) with respect to both \( w \) and \( n \) and can be expressed as a two-time correlation function:

\[ G(u, v) = \sum_{n=-\infty}^{\infty} \int dw e^{i u w + i v n} p(w, n) \]  

\[ = \langle e^{i u H_H(\tau) + i u N_H(\tau)} e^{-i u H(0) - i u N(0)} \rangle_{\rho}, \]

where the average \( \langle X \rangle_{\rho_c} = Tr X e^{-\beta H(0)} e^{\beta \mu N(0)}/Q_i \) is performed over the initial grand canonical state with \( Q_i \) being the grand canonical partition function of the initial state. Here the index \( H \) indicates operators in the Heisenberg picture given by \( O_H(\tau) = U^\dagger(\tau, 0) O(\tau) U(\tau, 0) \). Based on the micro-reversibility of the time evolution \( U(\tau, t) = \Theta^\dagger U_b(t - \tau, 0) \Theta \) relating the time evolution \( U \) of the original process to the time evolution \( U_b \) for the reversed protocol by means of the anti-unitary time-reversal operator \( \Theta \), one obtains the following relation between characteristic functions of the forward and the backward process

\[ Q_i G(u, v) = G_b(-u + i \beta, -v - i \beta \mu) Q_f. \]  

Taking the inverse Fourier transform of this relation leads to Eq. (9), where \( \beta \Delta \Phi = -(\ln Q_f - \ln Q_i) \).

### IV. PROTOCOL

The protocol according to which the trap curvature is changed specifies the time-dependent change of the frequency \( \omega(t) \) within a time interval \([0, \tau]\). In the present investigation we assume that it consists in an adiabatically slow change connecting the boundary values

\[ \omega(0) = \omega, \quad \omega(\tau) = (1 + \gamma) \omega. \]  

A positive (negative) value of \( \gamma \) indicates that the system is compressed (expanded) during the protocol. With the adiabatic variation of the frequency the occupation numbers \( n_\ell \) of the \( \ell \)'s single particle eigenstates remain unchanged such that the time evolution operator takes the form

\[ U(t, 0) = \sum_{\{n_\ell\}} \langle \{n_\ell\}, t | \{n_\ell\}, 0 \rangle, \]

where \( \{|n_\ell\}, t \rangle = |n_0, n_1, \cdots ; t \rangle \) with \( \sum_\ell n_\ell = N \) is an eigenfunction of the \( N \)-particle Hamiltonian \[^4\]^ and hence a solution of

\[ \mathcal{H}(t)|\{n_\ell\}, t \rangle = E(t)|\{n_\ell\}, t \rangle \]  

\[ E(t) = \sum_\ell \epsilon_\ell(t) n_\ell. \]

The corresponding \( N \)-particle eigenvalue \( E(t) \) is expressed in terms of the single-particle energy eigenvalues \( \epsilon_\ell(t) \) given by Eq. (4) and the occupation numbers \( n_\ell \) of these states. We consider this adiabatic protocol for the sake of simplicity. Although the shape of the work PDF will depend on the details of the specific protocol their relevant qualitative features leading to a diverging EWA are expected to be independent of those details.
V. ANALYTIC PROPERTIES OF THE CHARACTERISTIC FUNCTION

Using Eqs. (13) and (14), we obtain for the Hamiltonian and the number operator in the Heisenberg picture at the final time \( \tau \) of the protocol

\[
\begin{align*}
H_H(\tau) &= \sum_{\{ n_\ell \}} \langle \{ n_\ell \}, 0 \rangle \{ \{ n_\ell \}, 0 \}, \\
N_H(\tau) &= \sum_{\{ n_\ell \}} \langle \{ n_\ell \}, 0 \rangle \{ \{ n_\ell \}, 0 \} = N(0),
\end{align*}
\]

where \( \sum_{\{ n_\ell \}} \) denotes the summation under the constraint \( \sum_\ell n_\ell = N \). As a consequence of the number conservation for the considered protocol, the characteristic function becomes independent of the variable \( v \) which is conjugate to the number change \( n \). Hence, we get \( G(u, v) = G(u) \), implying \( p(w, n) = p(w)\delta_{n,0} \) for the joint probability.

Since all operators entering the characteristic function \( \ln Q (n) \) under the trace are diagonal with respect to the eigenbasis of the initial Hamiltonian, all of them commute with each other and it therefore is straightforward to write

\[
G(u) = \mathcal{Q}_l^{-1} \sum_{N=0}^{\infty} \sum_{\{ n_\ell \}} \prod_{\ell} e^{i u \xi_\ell n_\ell} e^{-i (u - i \gamma) \xi_\ell(0) n_\ell} z^{n_\ell} = \mathcal{Q}_l^{-1} \prod_{l=0}^{\infty} \left[ 1 - e^{(iu - \beta - \gamma) \omega_\ell (l+3/2)} \right]^{-g(l)}.
\]

Here the product on the right hand side of the first line extends over the triple index \( \ell = (\ell_x, \ell_y, \ell_z) \). The restriction in the second sum on the right hand side of the first line is lifted by the first sum over \( N \). Therefore all sums over the \( n_\ell \) can be performed in closed form leading to the expression in the second line. Because of the degeneracy of the single particle energies \( \xi_\ell(t) \) having the same value for a given \( l = \ell_x + \ell_y + \ell_z \), see Eq. (14), the product in the second line can be taken for \( l = 0, 1, 2, \ldots \). The degree of the degeneracy of the single particle energies \( \xi_\ell(t) \) is given by \( g(l) = (l+1)(l+2)/2 \).

Since \( u \) and \( \gamma \) only enter in the combination \( u \gamma \) the work PDF, which is given by the inverse Fourier transform of the characteristic function through Eq. (10), depends on \( w \) and \( \gamma \) in terms of the ratio \( w/\gamma \):

\[
p(w) = \frac{1}{|\gamma|} f(w/\gamma),
\]

where \( f(x) = (2\pi)^{-1} \int_0^\infty e^{-ix}\xi G(\xi) \) with \( \xi = u \gamma \). This leads to a symmetry relation between the work PDFs for compression (\( \gamma > 0 \)) and expansion (\( \gamma < 0 \)):

\[
p(w)|_{\gamma > 0} = p(-w)|_{\gamma < 0}.
\]

In presenting numerical results of the PDFs, we only consider the expansion case for a specific value of \( \gamma \). However, thanks to the relations, Eqs. (17) and (18), PDFs for other cases not shown here can be visualized.

It is worthwhile here to mention that the convergence of \( \langle e^{-\beta w} \rangle_{ge} \) is determined by the structure of the singularities of the characteristic function. The poles of \( G(u) \) are located along the imaginary axis in the complex plane of \( u = u' + iu'' \), where \( G(iu'')^{-1} = 0 \), yielding

\[
(u'')^l = -\frac{\beta (\xi_l(0) - \mu)}{\epsilon_l(0) \gamma}, \quad l = 1, 2, \ldots
\]

If \( \gamma > 0 \), then all poles are located in the lower half-plane \( u'' < 0 \) so that a divergence of \( G(iu') = \langle e^{-\beta u''} \rangle_{ge} \) can only occur in the unphysical regime of negative temperatures. On the other hand, for \( \gamma < 0 \) all pole positions are at positive values, \( u'' > 0 \). If the inverse temperature lies below the smallest pole position \( u'' = \beta (\xi_l(0) - \mu)/\gamma \) the EWA \( \langle e^{-\beta w} \rangle_{ge} \) is finite. The opposite case leads to a divergent EWA. Hence the condition for a finite EWA becomes

\[
(1 + \gamma)\epsilon_0(0) > \mu.
\]

Since \( (1 + \gamma)\epsilon_0(0) = \epsilon_0(\tau) \) is the single particle ground state in the trap at the end of the protocol this condition is identical with the condition of the existence of the hypothetical equilibrium state as explained at the end of Sec. II.

So far we have considered the chemical potential and the temperature as independent thermodynamic variables characterizing the initial state. In many practical applications it is more convenient to consider the average particle number as prescribed instead of the chemical potential. As a consequence the chemical potential then becomes a function of the average particle number and temperature and also the existence of a finite EWA then depends on temperature.

VI. ASYMPTOTIC RESULTS

In the extreme temperature limits, analytic forms of the work PDF can be obtained.

A. High temperatures

At high temperatures, the ground state energy is much smaller than the thermal energy, \( \epsilon_0 \ll k_B T \) and hence \( \beta_0 \) serves as expansion parameter. The mean number of the particles and the initial grand partition function then are approximately given by

\[
N_{av} \approx z \sum_{l=0}^{\infty} g(l) e^{-\beta \epsilon_l(0)} \approx \frac{e^{\beta \mu}}{(\beta_0)^3},
\]

\[
\ln Q_i = -\sum_{l=1}^{\infty} g(l) \ln[1 - ze^{-\beta \epsilon_l(0)}] \approx N_{av}.
\]
The second line gives the equation of states of an ideal gas. In the high temperature regime, positively or negatively large values of the work have highest probability for widening or narrowing, respectively, the trap. It is therefore sufficient to consider the contributions of the small values of $u$ to the characteristic function yielding:

$$\ln G_{\text{ht}}(u) = \frac{e^{\beta u}}{(\beta \hbar \omega)^3} \left[ -1 + \frac{1}{1 - i \gamma u / \beta} \right].$$

This asymptotic high temperature result agrees with the characteristic function of work for a classical system of non-interacting particles in a harmonic trap that initially stays in equilibrium with a reservoir and then experiences an adiabatic change of the trap curvature, see the appendix. The PDF corresponding to the high temperature limit characteristic function is not known analytically. However, in the case of small curvature changes, i.e. $|\gamma| \ll 1$ one can perform an expansion in powers of $\gamma$, leading to:

$$\ln G_{\text{ht}}(u) \approx \frac{e^{\beta u}}{(\beta \hbar \omega)^3} (3i \gamma u / \beta - 6 \gamma^2 u^2 / \beta^2).$$

Within this approximation the work average and its standard deviation become:

$$\langle u \rangle = \frac{3 N_{av} \gamma}{\beta},$$

$$\sigma_u^2 = \frac{4 \gamma^2}{\beta}. \quad (24)$$

The corresponding Gaussian distribution function of the work is then given by

$$p(w) = \frac{1}{\sqrt{2\pi \sigma_u^2}} \exp \left[ -\frac{(w - \langle w \rangle)^2}{2\sigma_u^2} \right]. \quad (25)$$

As shown in Fig. 2(a), this PDF obtained for high temperatures and small curvature deformations is in good agreement with the numerical evaluation of the PDF to be detailed in the next section. In the high temperature approximation, (25) the EWA becomes

$$\ln \langle e^{-\beta u} \rangle_{gc} \approx -3 N_{av} \gamma (1 - 2\gamma). \quad (26)$$

On the other hand, the grand canonical partition function of the hypothetical equilibrium state reads up to the second order in $\gamma$

$$\ln Q_f = - \sum_l q(l) \ln[1 - z e^{-\beta(1 + \gamma)(l + \epsilon_0)}]$$

$$\approx N_{av} (1 - 3\gamma + 6\gamma^2).$$

This together with $Q_i$ in Eq. (21) leads to $\ln [Q_f / Q_i] = \langle e^{-\beta u} \rangle_{gc}$, validating the Jarzynski equality, Eq. (2), within the Gaussian approximation. In passing we note that this need not be expected since the Gaussian approximation often fails to describe the wings of the work distribution with sufficient accuracy to conform with the Jarzynski equality [20].

![Figure 2](image-url)
end and the beginning of the protocol, each of which being evaluated at sufficiently low temperatures such that other than the ground state contributions can be neglected. Hence, the Jarzynski equality also holds for the approximate low temperature work PDF [23]. Note that for protocols leading to a ground state \( \epsilon_0(\tau) \) less than the chemical potential \( \mu \) formally leads to the nonsensical result of a negative EWA, indicating the actual divergence of the sum representing this average. Finally we note that for small values of the deformation parameter \( \gamma \) the spacing between the allowed values of the work becomes smaller suggesting to approximate the discrete work distribution by a continuous PDF which can be written as a generalized exponential PDF

\[
p(w) = \frac{1}{[\langle w \rangle]} e^{-w\langle w \rangle} \Theta(\gamma w), \tag{30}
\]

where \( \Theta(x) \) denotes the Heaviside step function. The average work \( \langle w \rangle \) follows from Eq. (29) as

\[
\langle w \rangle = \gamma \epsilon_0(0) \frac{ze^{-\beta \epsilon_0(0)}}{1 - ze^{-\beta \epsilon_0(0)}}. \tag{31}
\]

The sign of the average work is determined by that of \( \gamma \): Compressing the trap leads to positive, widening to negative work. In accordance with Eq. (20) there is no restriction for the existence of the EWA in the compression case. For widening though the characteristic scale on which the exponential distribution decays must be small enough that the increase of the exponentiated work \( e^\beta w \) for negative \( w \) is overcompensated and a finite EWA exists. The quantitative condition \( \beta |\langle w \rangle| < 1 \) following from (31) is identical with the condition implied by the existence of the hypothetical equilibrium state, \( \epsilon_0(0) > \mu \).

VII. NUMERICAL RESULTS

In order to investigate the behavior of the work PDFs in the intermediate temperature regime, we numerically evaluated the characteristic function in Eq. (10) and obtained the work PDF by means of an inverse transform algorithm proposed by Danielson and Lanczos [21]. Figure 3(a) displays the PDFs for \( \gamma = 0.9 \) and \( N_{av} = 100 \) at various temperatures. At \( T = 1.7T_c \) (see the curve labeled by E), the work PDF exhibits a decay that, on the logarithm scale, is faster than linear. At lower temperatures, the PDF becomes negatively skewed developing a more pronounced tail in the region of large negative work. At the extremely low temperature, \( T = 0.1T_c \) (labeled by A in Fig. 3), the PDF approaches the generalized exponential distribution, Eq. (30). The overall feature of this temperature dependence is confirmed also for smaller average particle numbers \( N_{av} = 10 \), the PDFs of which are shown in the panel (b).

As mentioned, the divergence of the EWA sets in when the ground state energy at the end of the work protocol is identical to the chemical potential of the reservoir. Figure 4 (a) displays the critical line determined by \( \gamma_c \), \( \epsilon_0 = \mu - \epsilon_0 \) for a given average number of particles. The hypothetical equilibrium state exists only in the region \( \gamma > \gamma_c \) of Fig. 4 (a). This is the case when the work is done by compressing the potential \( \gamma > 0 \) but also in the limit of high temperatures. On the other
hand, upon expanding the potential the EWA diverges at low temperatures. The key signature of this divergence is reflected in the tail of the PDF at negative work values. This property of the PDF can be conveniently quantified by the parameter

\[ \alpha = -\beta + \left( \frac{\partial \ln p(w)}{\partial w} \right)_{w=w_c}, \]  

(32)

which determines the convergence rate of the integral \( \int_{-\infty}^{w_c} dw e^{-\beta w} p(w) \). In our numerical investigation we chose \( w_c \) as the negative work for which the probability reaches the smallest possible value \( p(w_c) = 10^{-13} \) within the numerical precision of our calculations. Fig. 4(b) displays the high temperature region the\( \langle \alpha \rangle \) values for PDFs whose negative work tails approach an exponential behavior such that a reliable value of \( \alpha \) can be assigned. The temperatures in Fig. 4(a) indeed coincide with the instability regions given by the parameter \( \alpha \).

\[ \langle \alpha \rangle = \frac{1}{\beta} \ln \left( \frac{\int_{-\infty}^{w_c} dw e^{-\beta w} p(w)}{p(w_c)} \right). \]

In the intermediate regime the numerical results illustrate the transition between the extreme temperature regimes, which are in good agreement with numerical results. In the intermediate regime the numerical results illustrate the transition between the extreme temperature cases. As a quantitative measure for the decay of the PDFs we examined the decay rate \( \alpha \) of the characteristic function, Eq. (10), and the characteristic function becomes

\[ G(u) = Q^{-1} \sum_{N} e^{\beta \mu N} \text{Tr}_N e^{i u H_N} e^{-\beta H} \]

\[ = Q^{-1} \left( \sum_{N} e^{\beta \mu N} Z_N g_N(u) \right), \]

(31)

where \( Z_N \) is the canonical partition function of the \( N \)-particle system, and \( g_N(u) \) is the characteristic function of work for the \( N \)-particle system with initial canonical equilibrium state. In the particular case of non-interacting Boltzmann particles, the canonical \( N \) particle partition function can be expressed by the single-particle partition function \( Z_s \) as \( Z_N = (Z_s)^N / N! \) similarly the canonical \( N \)-particle generating function in terms of the one-particle generating function \( g_s(u) \) as \( g_N(u) = [g_s(u)]^N \). Using Eq. (31) and summing up the series, one obtains the characteristic function for the classical particles,

\[ G_c(u) = \exp \left[ e^{\beta \mu Z_s} (g_s(u) - 1) \right]. \]

(32)

For the example of particles subject to a three-dimensional isotropic harmonic potential undergoing a change of its curvature, the single-particle characteristic function becomes

\[ g_s(u) = \left\{ \int \frac{dp dq}{Z_s h} e^{i u [H(p(\tau), q(\tau), t) - H(p, q, 0)]} e^{-\beta H(p, q, 0)} \right\}^3, \]

(33)

where \( h \) is Planck’s constant. In the particular case of an adiabatically slow change of the potential curvature the time dependent Hamiltonian can be expressed in terms of the action \( I \) to yield

\[ H(p(t), q(t), t) = \frac{1}{2m} p(t)^2 + \frac{m}{2} \omega^2(t) q(t)^2 = \omega(t) I, \]

(34)

With the invariance of the action under adiabatic changes we get

\[ H(p(\tau), q(\tau), \tau) = H(p, q, 0) = (\omega(\tau) - \omega(0)) I = \gamma \omega I. \]

(35)

\[ \langle \alpha \rangle = \frac{1}{\beta} \ln \left( \frac{\int_{-\infty}^{w_c} dw e^{-\beta w} p(w)}{p(w_c)} \right). \]
Combined with \( \int dpdq = 2\pi \int_0^\infty dI \), this gives
\[
Z_s g_s(u) = \hbar^{-3} \left[ \int_0^\infty dI e^{-(\beta - i\gamma u)\omega I} \right]^3
\]
\[
= \frac{1}{(\beta - i\gamma u)^3(\hbar\omega)^3},
\]
and \( Z_s = 1/(\beta\hbar\omega)^3 \). Hence we find for the grand canonical characteristic function
\[
G_c(u) = \exp \left\{ \frac{e^{\beta\mu}}{(\beta\hbar\omega)^3} \left[ \frac{1}{(1 - i\gamma u/\beta)^3} - 1 \right] \right\},
\]
which coincides with the quantum expression of characteristic function at high temperatures, Eq. (22).

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FIG. 4: (a) Phase diagram depicting the region of existence of the hypothetical grand canonical state in the $\gamma - T/T_c$ plane. The borders separating the two regions of existence (II) and nonexistence (I) are depicted by a solid line for $N_{av} = 100$ and by a dotted line for $N_{av} = 10$. Compression ($\gamma > 0$) belongs to the region II irrespective of the temperature. If the potential is expanded the hypothetical equilibrium ceases to exist and region I is entered provided the temperature is low enough. At the expansion factor $\gamma = -0.1$ (dotted horizontal line), the region I is entered at $T \approx 0.93T_c$ for $N_{av} = 100$ and at $T \approx 0.77T_c$ for $N_{av} = 10$. The points A, B, C, D and E (crosses) correspond to the accordingly marked work PDFs that are displayed in Fig. 3. The convergence measure $\alpha$ introduced in Eq. (32) is displayed in panel (b) as a function of $T/T_c$ for $\gamma = -0.1$ and for $N_{av} = 100$ (⋄) and $N_{av} = 10$ (◦). The temperature values at which $\alpha$ changes the sign indicate the transition between finite and divergent EWA in agreement with the corresponding temperature values read off from panel (a). The vertical lines refer to the temperatures of the points B and C. For $N_{av} = 10$, the crossing points with the lines corresponding to B and C give positive and negative $\alpha$ values, respectively, in accordance with panel (a). For $N_{av} = 100$ both points yield positive $\alpha$ values in agreement with panel (a).