Thermodynamic equivalence of certain ideal Bose and Fermi gases

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We show that the recently discovered thermodynamic “equivalence” between noninteracting Bose and Fermi gases in two dimensions, and between one-dimensional Bose and Fermi systems with linear dispersion, both in the grand-canonical ensemble, are special cases of a larger class of equivalences of noninteracting systems having an energy-independent single-particle density of states. We also conjecture that the same equivalence will hold in the grand-canonical ensemble for any noninteracting quantum gas with a discrete ladder-type spectrum whenever \[ \frac{\sigma \Delta}{Nk_B T} \approx 0. \]
where \( N \) is the average particle number and \( \sigma \) is its standard deviation, \( \Delta \) is the level spacing, \( k_B \) is Boltzmann’s constant, and \( T \) is the temperature.

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I. INTRODUCTION

There has been considerable recent interest in surprising thermodynamic “equivalences” between certain ideal Bose and spinless Fermi gas systems, including nonrelativistic free particles in two dimensions \(^1\) and between one-dimensional particles with a linear, sound-like dispersion relation. \(^2\) Both results are valid in the grand-canonical ensemble, and assert that the Helmholtz free energies \( F \) and \( B \) of the Fermi and Bose systems, respectively, are simply related by

\[ F(T, V, N) - B(T, V, N) = \frac{N^2}{2C}, \]

where \( C \) is a constant that may depend on the system volume \( V \), but is independent of temperature \( T \) and the mean particle number \( N \). The Bose and Fermi systems are assumed to have identical single-particle Hamiltonians, and have the same \( T, V, \) and \( N \).

There are several immediate consequences of Eq. (1), including:

a. The entropies of the Fermi and Bose systems are identical,

\[ S_F(T, V, N) = S_B(T, V, N); \]

b. Their internal energies differ by a temperature-independent constant, namely

\[ U_F(T, V, N) - U_B(T, V, N) = \frac{N^2}{2C}; \]

c. The constant-volume heat capacities are identical;

d. The chemical potentials are simply shifted by a temperature-independent constant,

\[ \mu_F(T, V, N) - \mu_B(T, V, N) = \frac{N}{C}; \]
e. The thermodynamic potentials are connected by a relation opposite to (1),

\[ \Omega_F(T, V, N) - \Omega_B(T, V, N) = \frac{N^2}{2C}; \]
f. The pressures of the Fermi and Bose gases satisfy

\[ P_F(T, V, N) - P_B(T, V, N) = \frac{N^2}{2CV}, \]

and again differ only by a temperature-independent constant.

These results explain and considerably extend isolated thermodynamic relations that were discovered some time ago by May.\(^3\)

In this paper we demonstrate that the equivalence defined in Eq. (1) holds whenever the single-particle density of states (DOS) is independent of energy, for which the systems considered in Refs. \(1,2,3\) are special cases. We then extend recent results of Schmidt and Schnack \(^4\) and of Crescimanno and Landsberg \(^5\) on harmonically confined Bose and Fermi gases in one dimension to further enlarge the class of equivalences to include any ideal quantum gas with a discrete ladder-type spectrum, in the limit

\[ \frac{\sigma \Delta}{Nk_B T} \to 0. \]

Here \( N \) is the mean particle number, \( \sigma \) is the standard deviation in particle number about \( N \), \( \Delta \) is the energy-level spacing, \( k_B \) is Boltzmann’s constant, and \( T \) is the temperature. The condition (7) requires that either (i) the particle number is conserved, (ii) the number of particles is very large, (iii) the temperature is very high, (iv) the spectrum is continuous, or any combination of these possibilities.
II. THERMODYNAMIC EQUIVALENCE AND THE DENSITY OF STATES

We begin by writing the grand-canonical partition function of an arbitrary noninteracting Bose or Fermi system as

\[ Z = \prod_\alpha \sum_{N_\alpha} e^{-\beta(\epsilon_\alpha - \mu)N_\alpha}. \]  

(8)

Here \( \alpha \) labels the quantum states of a single Bose or spinless Fermi particle with spectrum \( \epsilon_\alpha \), and \( \beta \equiv 1/k_B T \). The occupation numbers \( N_\alpha \) take the values \( N_\alpha = 0, 1, 2, \cdots \) for bosons and \( N_\alpha = 0, 1 \) for fermions. The thermodynamic potential \( \Omega \equiv F - \mu N \) is given by

\[ \Omega = -\frac{1}{\beta} \ln Z. \]  

(9)

Because the average number of particles is required to be the same for the Bose and Fermi cases, their chemical potentials \( \mu \) in Eq. (9) are different. The relations between \( \mu_B \), \( \mu_F \), and \( N \), are determined by

\[ \sum_\alpha n_B(\epsilon_\alpha - \mu_B) = \sum_\alpha n_F(\epsilon_\alpha - \mu_F) = N, \]  

(10)

where

\[ n_B(x) \equiv \frac{1}{e^{\beta x} - 1} \quad \text{and} \quad n_F(x) \equiv \frac{1}{e^{\beta x} + 1} \]  

(11)

are the Bose and Fermi distribution functions.

Next we define a single-particle DOS according to

\[ g(\epsilon) \equiv \sum_\alpha \delta(\epsilon - \epsilon_\alpha), \]  

(12)

which gives the number of energy levels per unit energy, as a function of \( \epsilon \). In a translationally invariant system, \( g(\epsilon) \) scales linearly with system volume \( V \). In terms of the DOS, we have

\[ \Omega_B = \frac{1}{\beta} \int_{-\infty}^\infty d\epsilon g(\epsilon) \ln(1 - e^{-\beta \epsilon} z_B) \]  

(13)

and

\[ \Omega_F = -\frac{1}{\beta} \int_{-\infty}^\infty d\epsilon g(\epsilon) \ln(1 + e^{-\beta \epsilon} z_F), \]  

(14)

where \( z_B \equiv e^{\beta \mu_B} \) and \( z_F \equiv e^{\beta \mu_F} \) are the Bose and Fermi fugacities. Furthermore, condition (11) can be written as

\[ \int_{-\infty}^\infty d\epsilon \frac{g(\epsilon)}{e^{\beta \epsilon} z_B - 1} = \int_{-\infty}^\infty d\epsilon \frac{g(\epsilon)}{e^{\beta \epsilon} z_F + 1}. \]  

(15)

The expressions (13), (14), and (15), are valid for any noninteracting quantum gas.

We assume that spectrum is bounded from below, and that the DOS is a constant, \( C \), independent of energy, above that minimum. Without loss of generality we can take the minimum to be at \( \epsilon = 0 \). Then

\[ g(\epsilon) = C \Theta(\epsilon), \]  

(16)

where \( \Theta(\epsilon) \) is the unit step function. The most common example of a DOS of the form (16) occurs for free nonrelativistic particles of mass \( m \) in two dimensions, in which case

\[ C = \frac{2m}{\pi \hbar^2}. \]  

(17)

However, there are other situations where (16) holds as well, including noninteracting particles moving in one dimension with a linear dispersion \( \epsilon(k) \propto |k| \), and also for particles moving in three dimensions with cubic dispersion \( \epsilon(k) \propto |k|^3 \). These cases were noted earlier by Pathria. Furthermore, we note that the equivalence (11) would not apply to two-dimensional systems moving in the potential of a corrugated surface or to ideal lattice gas models.

Assuming (16), we can immediately obtain

\[ \Omega_B = -\frac{C}{\beta^2} \text{Li}_2(z_B) \]  

(18)

and

\[ \Omega_F = -\frac{C}{\beta^2} \text{Li}_2(-z_F), \]  

(19)

where \( z_B = 1 - e^{-\beta N/C} \) and \( z_F = e^{\beta N/C} - 1 \). Here \( \text{Li}_2(x) \) is Euler’s dilogarithm function. Furthermore, from Eq. (15), we have \( \mu_F - \mu_B = N/C \) and \( z_F = z_B/(1 - z_B) \). These relations, along with the identity

\[ \text{Li}_2(x) + \text{Li}_2(\frac{1}{1-x}) = -\frac{1}{2} \ln(1-x)^2, \]  

(20)

directly lead to the equivalence stated in (11). The thermodynamic equivalence evidently applies to any noninteracting quantum gas with a constant DOS.

It is also instructive to directly demonstrate the equivalence of the entropies: For a system with a constant DOS of the form (16), the Bose and Fermi entropies are

\[ S_B = -C k_B \int_0^\infty d\epsilon \left[ n_B(\epsilon - \mu_B) \ln[n_B(\epsilon - \mu_B)] - \left[1 + n_B(\epsilon - \mu_B)\right] \ln[1 + n_B(\epsilon - \mu_B)] \right] \]  

(21)

and

\[ S_F = -C k_B \int_0^\infty d\epsilon \left[ n_F(\epsilon - \mu_F) \ln[n_F(\epsilon - \mu_F)] + \left[1 - n_F(\epsilon - \mu_F)\right] \ln[1 - n_F(\epsilon - \mu_F)] \right]. \]  

(22)

Changing the integration variable in the Bose case to \( w = e^{\beta(\epsilon - \mu_B)} - 1 \), and in the Fermi case to \( w = e^{\beta(\epsilon - \mu_F)} \), leads to

\[ S_B = C k_B^2 \text{Li} \int_{z_B - 1}^\infty dw \left[ \ln(1+w) - \ln w \right] \]  

(23)
and

\[
S_F = \frac{C}{\hbar^2 T} \int_{\frac{\mu}{kT}}^{\infty} dw \left[ \ln(1 + w) - \frac{\ln w}{1 + w} \right].
\]  

(24)

Notice that the statistics dependence enters only in the lower integration limits. Because the average particle numbers are the same, these lower limits coincide and thus the Fermi and Bose entropies are identical.

III. 1D QUANTUM GASES IN HARMONIC POTENTIALS AND AN EXTENDED EQUIVALENCE

It is interesting to consider whether a constant DOS is necessary for the equivalence defined in Eq. (1). In particular, does it apply to a system with a discrete ladder-type spectrum of the form

\[
\epsilon_n = n \Delta, \quad n = 0, 1, 2, 3, \ldots
\]  

(25)

where \( \Delta \) is the level spacing, which reduces to the case considered in Sec. II in the limit \( \Delta \to 0 \). In this section we demonstrate that the equivalence does still hold, in the grand-canonical ensemble, for noninteracting gases with the spectrum (25), in the limit \( N \to \infty \), and also in the canonical ensemble for any \( N \).

In Figs. 1 and 2, we show the Helmholtz free energy per particle, numerically calculated in the grand-canonical ensemble, for 1D quantum gases in a harmonic potential with level spacing \( \Delta \). The free energies and temperatures are plotted in units of \( \Delta \). In these figures, the solid curves are for \( N = 1000 \) and the dashed curves are for \( N = 10 \). In Fig. 3, the difference between the Fermi and Bose free energies are given as a function of temperature, with \( F_F \) shifted by the Fermi ground-state energy \( E_N \) [defined below in Eq. (30)] for convenience.

For small \( N \) (dashed curve in Fig. 3), the free energies clearly do not differ by a temperature-independent constant. However, as \( N \) becomes larger (solid curve), the equivalence does apply. These numerical results suggest that when particle-number fluctuations become negligible, the equivalence holds. To establish this result, we use the fact that in the large-\( N \) limit, the grand-canonical free energy approaches the canonical free energy (shown in Figs. 1 and 2 as dotted curves), and that the equivalence holds exactly in the canonical ensemble.

Writing the grand-canonical partition function \( Z \) in terms of the canonical partition functions \( Z_N \) according to

\[
Z = \sum_{N=1}^{\infty} Z_N z^N, \quad z \equiv e^{\beta \mu},
\]  

(26)

where \( z \) is the fugacity, leads to

\[
Z_N = \frac{1}{N!} \left( \frac{\partial^N Z}{\partial z^N} \right)_{z=0}.
\]  

(27)

For Bose (\( \zeta = 1 \)) and Fermi (\( \zeta = -1 \)) particles with spectrum (25), the grand-canonical partition function is

\[
Z = \exp \left[ -\zeta \sum_{n=0}^{\infty} \ln \left( 1 - \zeta b^n z \right) \right] \quad \text{with} \quad b \equiv e^{-\beta \Delta},
\]  

(28)

from which we obtain

\[
Z_N = e^{-\beta E_N} \times \prod_{j=1}^{N} \left( \frac{1}{1 - b^j} \right).
\]  

(29)

Here

\[
E_N = \begin{cases} 
0 & \text{for bosons} \\
\frac{N(N-1)}{2} \Delta & \text{for fermions}
\end{cases}
\]  

(30)

is the ground-state energy of \( N \) particles. The result in Eq. (29) was also obtained by Schmidt and Schnack using related methods.
According to Eq. (29), the canonical free energy for \( N \) particles is simply
\[
F_N = E_N + k_B T \sum_{j=1}^{N} \ln \left( 1 - e^{-\beta \Delta j} \right),
\]
the Bose and Fermi cases simply differing by the constant \( E_N \). The second term in (31) does not depend on the quantum statistics parameter \( \zeta \). Schmidt and Schnack\(^4\) also recognized the partial equivalence between 1D ideal Bose and Fermi gases in harmonic confining potentials. Later, Crescimanno and Landsberg\(^5\) showed that the physical origin of that equivalence in the canonical ensemble is the exact mapping between the many-particle excitation spectra of both systems.

Finally, we note that the thermodynamic equivalence with the spectrum\(^2\) also trivially holds in the \( T \rightarrow \infty \) limit, because in this limit the systems become classical. Therefore we conjecture that the equivalence defined in Eq. (1) will hold in the grand-canonical ensemble for any noninteracting quantum gas with a discrete ladder-type spectrum, whenever the quantity
\[
\frac{\sigma \Delta}{N k_B T}
\]
is small, where \( N \) is the average particle number and \( \sigma \) is its standard deviation about \( N \). This ratio roughly characterizes the magnitude of energy fluctuations caused by the exchange of particles with the environment—if allowed—relative to the thermal energy. We conclude that the (partial) thermodynamic equivalence discovered by Lee\(^1\) holds for ideal quantum gases with the spectrum \( \Delta = 0 \) whenever (i) the number of particles is strictly conserved, (ii) the number of particles becomes very large so that \( \sigma/N \rightarrow 0 \), (iii) \( T \rightarrow \infty \), (iv) \( \Delta \rightarrow 0 \), or when any combination of these criteria are fulfilled.

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1. M. H. Lee, Phys. Rev. E 55, 1518 (1997).
2. R. K. Pathria, Phys. Rev. E 57, 2697 (1998).
3. R. M. May, Phys. Rev. 135 A1515 (1964).
4. H.-J. Schmidt and J. Schnack, Physica A 260, 479 (1998).
5. M. Crescimanno and A. S. Landsberg, Phys. Rev. A 63, 35601 (2001).
6. L. D. Landau and E. M. Lifshitz, Statistical Physics, 3rd ed. (Pergamon Press, Oxford, 1980), Part 1.