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Thermodynamic equivalence of certain ideal Bose and Fermi gases

Kelly R. Patton[a], Michael R. Geller[a,*], Miles P. Blencowe[b]

[a]Department of Physics and Astronomy, University of Georgia, Athens, GA 30602-2451, USA
[b]Department of Physics and Astronomy, Dartmouth College, Hanover, NH 03755, USA

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Abstract

It has been established recently that there is an interesting thermodynamic "equivalence" between noninteracting Bose and spinless Fermi gases in two dimensions, and between one-dimensional Bose and Fermi systems with linear dispersion, both in the grand-canonical ensemble. These are known to be special cases of a larger class of equivalences of noninteracting systems having an energy-independent single-particle density of states (DOS). Furthermore, the thermodynamic equivalence has also been established for any noninteracting quantum gas with a discrete ladder-type spectrum in the *canonical* ensemble. Here we investigate the intriguing possibility that the equivalence for systems with a constant DOS is a special case of a more general equivalence between noninteracting Bose and Fermi gases with a discrete ladder-type spectrum in the grand-canonical ensemble, which reduces to the constant-DOS case when the level-spacing approaches zero. By direct numerical calculation of the Bose and Fermi grand-canonical free energies, we conclude that the grand-canonical equivalence does not apply to the ladder-spectrum case.

Keywords: Ideal Bose gas; Ideal Fermi gas

*Corresponding author. Tel.: +1 706 542 2834; fax: +1 706 542 2492.
E-mail address: mgeller@physast.uga.edu (M.R. Geller).

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1. 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, as discussed by Lee[1] [1], and between one-dimensional particles with a linear, sound-like dispersion relation, as discussed by Pathria [2]. Both results are valid in the grand-canonical ensemble, and assert that the Helmholtz free energies F_F and F_B of the Fermi and Bose systems, respectively, are simply related by

$$F_F(T, V, N) - F_B(T, V, N) = \frac{N^2}{2\mathscr{C}} , \tag{1}$$

where $\mathscr{C}$ is a constant that may depend on the system volume V, but is independent of the 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 (1), including:

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

$$S_F(T, V, N) = S_B(T, V, N) . \tag{2}$$

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

$$U_F(T, V, N) - U_B(T, V, N) = \frac{N^2}{2\mathscr{C}} . \tag{3}$$

(c) The constant-volume heat capacities are identical.

(d) The chemical potentials are shifted by a temperature-independent constant,

$$\mu_F(T, V, N) - \mu_B(T, V, N) = \frac{N}{\mathscr{C}} . \tag{4}$$

(e) The thermodynamic potentials are connected by a relation opposite to (1),

$$\Omega_F(T, V, N) - \Omega_B(T, V, N) = -\frac{N^2}{2\mathscr{C}} . \tag{5}$$

(f) The pressures of the Fermi and Bose gases satisfy

$$P_F(T, V, N) - P_B(T, V, N) = \frac{N^2}{2\mathscr{C} V} \tag{6}$$

and again differ only by a temperature-independent constant.

[1]Lee actually derives an equivalence between ideal gases having the same $N\lambda^2/V$, where λ is the thermal wavelength, allowing for the possibility of different T, V, and N.

These results explain and considerably extend thermodynamic relations that were discovered by May [3] some time ago. Anghel [4] has also recently shown that the thermodynamic equivalence applies to any noninteracting system having an energy-independent single-particle density of states (DOS).

The same equivalence holds between harmonically confined ideal Bose and Fermi gases in one dimension, where the spectrum is a discrete, uniformly spaced ladder, except that in this case the equivalence has been established only for the canonical ensemble. In the thermodynamic limit, these two ensembles are equivalent, but in a small system the differences can be significant. The equivalence in a one-dimensional harmonic potential was proved by Schmidt and Schnack [5] and also by Crescimanno and Landsberg [6]. It was also known from work on bosonization of the one-dimensional electron gas [7]. The following question naturally arises: could the equivalence for systems with a constant DOS be a special case of a more general equivalence between noninteracting Bose and Fermi gases with a discrete ladder-type spectrum in the grand-canonical ensemble, which reduces to the constant-DOS case when the level-spacing approaches zero? By direct numerical calculation of the Bose and Fermi grand-canonical free energies we find that this is *not* the case.

2. Thermodynamic equivalence and the density of states

To proceed, we rederive the grand-canonical equivalence in the constant-DOS case, using a method similar to that of Anghel [4]. We write the grand-canonical partition function of an arbitrary noninteracting Bose or Fermi system as

$$Z = \prod_{\alpha} \sum_{N_\alpha} \mathrm{e}^{-\beta(\varepsilon_\alpha - \mu)N_\alpha} \,. \tag{7}$$

Here α labels the quantum states of a single Bose or spinless Fermi particle with spectrum ε_α, and $\beta \equiv 1/k_{\mathrm{B}}T$. The occupation numbers N_α take the values $N_\alpha = 0, 1, 2, \ldots$ for bosons and $N_\alpha = 0, 1$ for fermions. The thermodynamic potential $\Omega \equiv F - \mu N$ is given by

$$\Omega = -\frac{1}{\beta} \ln Z \,. \tag{8}$$

Because the average number of particles is required to be the same for the Bose and Fermi cases, their chemical potentials μ in (7) are different. The relations between μ_{B}, μ_{F}, and N are determined by

$$\sum_{\alpha} n_{\mathrm{B}}(\varepsilon_\alpha - \mu_{\mathrm{B}}) = \sum_{\alpha} n_{\mathrm{F}}(\varepsilon_\alpha - \mu_{\mathrm{F}}) = N \,, \tag{9}$$

where

$$n_{\mathrm{B}}(x) \equiv \frac{1}{\mathrm{e}^{\beta x} - 1} \quad \text{and} \quad n_{\mathrm{F}}(x) \equiv \frac{1}{\mathrm{e}^{\beta x} + 1} \tag{10}$$

are the Bose and Fermi distribution functions.

Next, we define a single-particle DOS according to

$$g(\varepsilon) \equiv \sum_{\alpha} \delta(\varepsilon - \varepsilon_{\alpha}) \,, \tag{11}$$

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

$$\Omega_{\mathrm{B}} = \frac{1}{\beta} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, g(\varepsilon) \, \ln(1 - \mathrm{e}^{-\beta\varepsilon} z_{\mathrm{B}}) \tag{12}$$

and

$$\Omega_{\mathrm{F}} = -\frac{1}{\beta} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, g(\varepsilon) \, \ln(1 + \mathrm{e}^{-\beta\varepsilon} z_{\mathrm{F}}) \,, \tag{13}$$

where $z_{\mathrm{B}} \equiv \mathrm{e}^{\beta\mu_{\mathrm{B}}}$ and $z_{\mathrm{F}} \equiv \mathrm{e}^{\beta\mu_{\mathrm{F}}}$ are the Bose and Fermi fugacities. Furthermore, condition (9) can be written as

$$\int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, \frac{g(\varepsilon)}{\mathrm{e}^{\beta\varepsilon} \, z_{\mathrm{B}}^{-1} - 1} = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, \frac{g(\varepsilon)}{\mathrm{e}^{\beta\varepsilon} \, z_{\mathrm{F}}^{-1} + 1} \,. \tag{14}$$

The expressions (12), (13), and (14), are valid for any noninteracting quantum gas.

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

$$g(\varepsilon) = \mathscr{C} \Theta(\varepsilon) \,, \tag{15}$$

where $\Theta(\varepsilon)$ is the unit step function. The most common example of a DOS of the form (15) occurs for free nonrelativistic particles of mass m in two dimensions, in which case

$$\mathscr{C} = \frac{mA}{2\pi\hbar^2} \,, \tag{16}$$

with A the system area. However, there are other situations where (15) holds as well, including noninteracting particles moving in one dimension with a linear dispersion $\varepsilon(k) \propto |k|$, and also for particles moving in three dimensions with qubic dispersion $\varepsilon(k) \propto |k|^3$. These cases were noted earlier by Pathria [2]. Furthermore, we note that the equivalence (1) would *not* apply to two-dimensional particles moving in the potential of a corrugated surface or to ideal lattice gas models. The equivalence is a property of the spectrum, not of the dimensionality. Also note that the thermodynamic limit is not required, only a smooth DOS of form (15).

Assuming (15), we obtain

$$\Omega_{\mathrm{B}} = -\frac{\mathscr{C}}{\beta^2} \, \mathrm{Li}_2(z_{\mathrm{B}}) \tag{17}$$

and

$$\Omega_{\mathrm{F}} = \frac{\mathscr{C}}{\beta^2}\,\mathrm{Li}_2(-z_{\mathrm{F}})\,, \tag{18}$$

where $z_{\mathrm{B}} = 1 - \mathrm{e}^{-\beta N/\mathscr{C}}$ and $z_{\mathrm{F}} = \mathrm{e}^{\beta N/\mathscr{C}} - 1$. Here $\mathrm{Li}_2(x)$ is Euler's dilogarithm function. Furthermore, from (14), we have $\mu_{\mathrm{F}} - \mu_{\mathrm{B}} = N/\mathscr{C}$ and $z_{\mathrm{F}} = z_{\mathrm{B}}/(1 - z_{\mathrm{B}})$. These relations, along with the identity

$$\mathrm{Li}_2(x) + \mathrm{Li}_2\left(\frac{x}{x-1}\right) = -\frac{1}{2}[\ln(1-x)]^2\,, \tag{19}$$

directly lead to the equivalence stated in (1). The thermodynamic equivalence evidently applies to any noninteracting quantum gas with a constant DOS [4].

It is also instructive to directly demonstrate the equivalence of the entropies: for a system with a constant DOS of the form (15), the Bose and Fermi entropies are [8]

$$\begin{aligned} S_{\mathrm{B}} = & -\mathscr{C}k_{\mathrm{B}} \int_0^\infty \mathrm{d}\varepsilon\,[n_{\mathrm{B}}(\varepsilon-\mu_{\mathrm{B}})\ln[n_{\mathrm{B}}(\varepsilon-\mu_{\mathrm{B}})] \\ & - [1+n_{\mathrm{B}}(\varepsilon-\mu_{\mathrm{B}})]\ln[1+n_{\mathrm{B}}(\varepsilon-\mu_{\mathrm{B}})]] \end{aligned} \tag{20}$$

and

$$\begin{aligned} S_{\mathrm{F}} = & -\mathscr{C}k_{\mathrm{B}} \int_0^\infty \mathrm{d}\varepsilon\,[n_{\mathrm{F}}(\varepsilon-\mu_{\mathrm{F}})\ln[n_{\mathrm{F}}(\varepsilon-\mu_{\mathrm{F}})] \\ & + [1-n_{\mathrm{F}}(\varepsilon-\mu_{\mathrm{F}})]\ln[1-n_{\mathrm{F}}(\varepsilon-\mu_{\mathrm{F}})]]\,. \end{aligned} \tag{21}$$

Changing the integration variable in the Bose case to $w = \mathrm{e}^{\beta(\varepsilon-\mu_{\mathrm{B}})} - 1$, and in the Fermi case to $w = \mathrm{e}^{\beta(\varepsilon-\mu_{\mathrm{F}})}$, leads to

$$S_{\mathrm{B}} = \mathscr{C}k_{\mathrm{B}}^2 T \int_{z_{\mathrm{B}}^{-1}-1}^{\infty} \mathrm{d}w \left[\frac{\ln(1+w)}{w} - \frac{\ln w}{1+w}\right] \tag{22}$$

and

$$S_{\mathrm{F}} = \mathscr{C}k_{\mathrm{B}}^2 T \int_{z_{\mathrm{F}}^{-1}}^{\infty} \mathrm{d}w \left[\frac{\ln(1+w)}{w} - \frac{\ln w}{1+w}\right]\,. \tag{23}$$

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

3. 1D Quantum gases in harmonic potentials

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

$$\varepsilon_n = n\Delta, \quad n = 0, 1, 2, 3, \ldots\,, \tag{24}$$

where Δ is the level spacing, which reduces to the case considered in Section 2 in the limit $\Delta \to 0$? This would imply that the equivalence proved by Schmidt and Schnack [5] and by Crescimanno and Landsberg [6] holds in the grand-canonical ensemble as well as the canonical one. However, we will show that this is not the case.

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 Δ. The free energies and temperatures are plotted in units of Δ. 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 (29)] 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. This makes sense given 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.

The equivalence in the canonical ensemble can be easily demonstrated as follows: writing the grand-canonical partition function Z in terms of the canonical partition functions Z_N according to

$$Z = \sum_{N=1}^{\infty} Z_N z^N, \quad z \equiv e^{\beta\mu}, \tag{25}$$

where z is the fugacity, leads to

$$Z_N = \frac{1}{N!} \left(\frac{\partial^N Z}{\partial z^N} \right)_{z=0}. \tag{26}$$

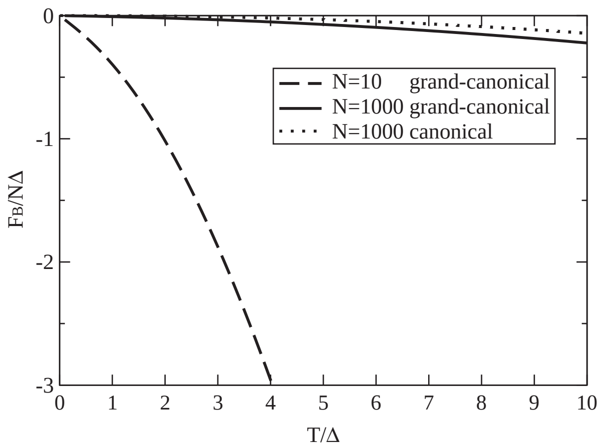

Fig. 1. Helmholtz free energy per particle for a 1D ideal Bose gas in a harmonic confining potential with level spacing Δ.

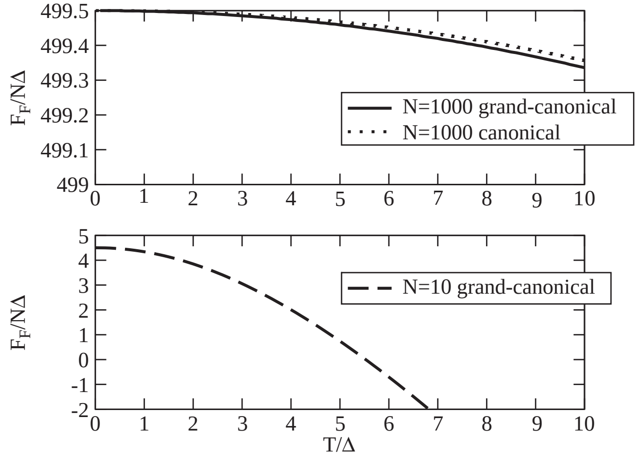

Fig. 2. Helmholtz free energy per particle for a 1D ideal Fermi gas in a harmonic confining potential with level spacing Δ.

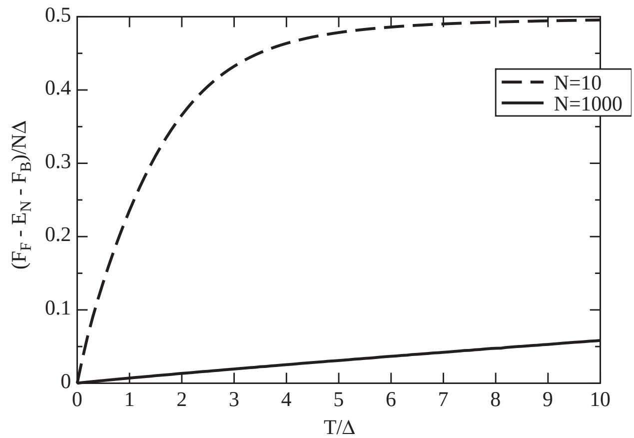

Fig. 3. Free energy difference per particle for ideal quantum gases in a harmonic confining potential. Here E_N is the ground-state energy of the Fermi system. Not shown is the difference in canonical ensemble case, which is exactly zero for any N.

For Bose ($\zeta = 1$) and Fermi ($\zeta = -1$) particles with spectrum (24), the grand-canonical partition function is

$$Z = \exp\left[-\zeta \sum_{n=0}^{\infty} \ln(1 - \zeta b^n z)\right], \quad \text{with } b \equiv e^{-\beta\Delta} , \tag{27}$$

from which we obtain

$$Z_N = \mathrm{e}^{-\beta E_N} \times \prod_{j=1}^{N} \left(\frac{1}{1-b^j} \right) . \tag{28}$$

Here

$$E_N \equiv \begin{cases} 0 & \text{for bosons} \\ \frac{N(N-1)}{2} \Delta & \text{for fermions} \end{cases} \tag{29}$$

is the ground-state energy of N particles. The result in (28) was also obtained by Schmidt and Schnack [5] using related methods.

According to (28), the canonical free energy for N particles is simply

$$F_N = E_N + k_{\mathrm{B}} T \sum_{j=1}^{N} \ln(1 - \mathrm{e}^{-\beta \Delta j}) , \tag{30}$$

the Bose and Fermi cases simply differing by the constant E_N. The second term in (30) does not depend on the quantum statistics parameter ζ. Schmidt and Schnack [5] also recognized the partial equivalence between 1D ideal Bose and Fermi gases in harmonic confining potentials. Later, Crescimanno and Landsberg [6] showed that the physical origin of this equivalence is the exact mapping between the many-particle excitation spectra of both systems, which is also known from work on bosonization [7].

We conclude that the thermodynamic equivalence for the case of a discrete, ladder-type spectrum does not hold in the grand-canonical ensemble for finite T and N. However, it must hold in the $T \to \infty$ limit, because in this limit the gas becomes classical, and it must hold in the $N \to \infty$ limit, because in this limit the particle-number fluctuations become negligible. Furthermore, we know that the equivalence holds in the $\Delta \to 0$ limit, because this is the constant-DOS case. It is therefore reasonable to conjecture that the equivalence defined in (1) will hold in the grand-canonical ensemble for any noninteracting quantum gas with a discrete ladder-type spectrum, whenever the ratio

$$\frac{\sigma \Delta}{N k_{\mathrm{B}} T} \tag{31}$$

is small, where N is the average particle number and σ 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. The (partial) thermodynamic equivalence discovered by Lee [1] holds for ideal quantum gases with the spectrum (24) whenever (i) the number of particles is strictly conserved, (ii) the number of particles becomes very large so that $\sigma/N \to 0$, (iii) $T \to \infty$, (iv) $\Delta \to 0$, or when any combination of these criteria are fulfilled.

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