PHYSICS 210A : EQUILIBRIUM STATISTICAL PHYSICS
HW ASSIGNMENT #4 SOLUTIONS

(1) For a noninteracting quantum system with single particle density of states $g(\varepsilon) = A\,\varepsilon^r$ (with $\varepsilon \geq 0$), find the first three virial coefficients for bosons and for fermions.

Solution :

We have

$$n(T,z) = \sum_{j=1}^{\infty} (\pm 1)^{j-1}\, C_j(T)\, z^j \qquad , \qquad p(T,z) = k_{\mathrm{B}}T \sum_{j=1}^{\infty} (\pm 1)^{j-1}\, z^j\, j^{-1}\, C_j(T)\, z^j \ ,$$

where

$$C_j(T) = \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\, e^{-j\varepsilon/k_{\mathrm{B}}T} = A\,\Gamma(r+1) \left(\frac{k_{\mathrm{B}}T}{j} \right)^{r+1} \ .$$

Thus, we have

$$\pm n v_T = \sum_{j=1}^{\infty} j^{-(r+1)}\, (\pm z)^j$$

$$\pm p v_T / k_{\mathrm{B}}T = \sum_{j=1}^{\infty} j^{-(r+2)}\, (\pm z)^j \ ,$$

where

$$v_T = \frac{1}{A\,\Gamma(r+1)\,(k_{\mathrm{B}}T)^{r+1}} \ .$$

has dimensions of volume. Thus, we let $x = \pm z$, and interrogate `Mathematica`:

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In[1]=  y = InverseSeries[x + x^2/2^(r+1) + x^3/3^(r+1) + x^4/4^(r+1) + O[x]^5]
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In[2]=  w = y + y^2/2^(r+2) + y^3/3^(r+2) + y^4/4^(r+2) + O[y]^5 .
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The result is

$$p = n k_{\mathrm{B}}T \left[1 + B_2(T)\, n + B_3(T)\, n^2 + \dots \right] \ ,$$

where

$$B_2(T) = \mp 2^{-2-r}\, v_T$$

$$B_3(T) = \left(2^{-2-2r} - 2 \cdot 3^{-2-r} \right) v_T^2$$

$$B_4(T) = \pm 2^{-4-3r}\, 3^{-r} \left(2^{3+2r} - 5 \cdot 3^r - 2^r\, 3^{1+r} \right) v_T^3 \ .$$

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(2) Consider a gas of particles with dispersion $\varepsilon(\boldsymbol{k}) = \varepsilon_0 \, |\boldsymbol{k}\ell|^{5/2}$, where ε_0 is an energy scale and ℓ is a length scale.

- (a) Find the density of states $g(\varepsilon)$ in $d = 2$ and $d = 3$ dimensions.

- (b) Find the virial coefficients $B_2(T)$ and $B_3(T)$ in $d = 2$ and $d = 3$ dimensions.

- (c) Find the heat capacity $C_V(T)$ in $d = 3$ dimensions for photon statistics.

Solution :

(a) For $\varepsilon(\boldsymbol{k}) = \varepsilon_0 \, |\boldsymbol{k}\ell|^\alpha$ we have

$$g(\varepsilon) = \int \frac{d^d k}{(2\pi)^d} \, \delta\big(\varepsilon - \varepsilon(\boldsymbol{k})\big) = \frac{\Omega_d}{(2\pi)^d} \int\limits_0^\infty dk \, k^{d-1} \, \frac{\delta\big(k - (\varepsilon/\varepsilon_0)^{1/\alpha}/\ell\big)}{\alpha \varepsilon_0 \ell^\alpha \, k^{\alpha-1}}$$

$$= \frac{\Omega_d}{(2\pi)^d} \, \frac{1}{\alpha \varepsilon_0 \ell^d} \left(\frac{\varepsilon}{\varepsilon_0}\right)^{\frac{d}{\alpha}-1} \Theta(\varepsilon) \, .$$

Thus, for $\alpha = \frac{5}{2}$,

$$g_{d=2}(\varepsilon) = \frac{1}{5\pi\varepsilon_0 \ell^2} \left(\frac{\varepsilon}{\varepsilon_0}\right)^{-1/5} \Theta(\varepsilon) \qquad , \qquad g_{d=3}(\varepsilon) = \frac{1}{5\pi\varepsilon_0 \ell^3} \left(\frac{\varepsilon}{\varepsilon_0}\right)^{1/5} \Theta(\varepsilon) \, .$$

(b) We must compute the coefficients

$$C_j = \int\limits_{-\infty}^\infty d\varepsilon \, g(\varepsilon) \, e^{-j\varepsilon/k_{\mathrm{B}}T} = \frac{\Omega_d}{(2\pi)^d} \, \frac{1}{\alpha \varepsilon_0 \ell^d} \int\limits_0^\infty d\varepsilon \left(\frac{\varepsilon}{\varepsilon_0}\right)^{\frac{d}{\alpha}-1} e^{-j\varepsilon/k_{\mathrm{B}}T}$$

$$= \frac{\Omega_d \, \Gamma(d/\alpha)}{(2\pi)^d} \, \frac{1}{\alpha \ell^d} \left(\frac{k_{\mathrm{B}}T}{j\varepsilon_0}\right)^{d/\alpha} \equiv j^{-d/\alpha} \, \lambda_T^{-d} \, ,$$

where

$$\lambda_T \equiv \frac{2\pi\ell}{\big[\Omega_d \, \Gamma(\tfrac{d}{\alpha})/\alpha\big]^{1/d}} \left(\frac{\varepsilon_0}{k_{\mathrm{B}}T}\right)^{1/\alpha} \, .$$

Then

$$B_2(T) = \mp \frac{C_2}{2 \, C_1^2} = \mp 2^{-\left(\frac{d}{\alpha}+1\right)} \, \lambda_T^d$$

$$B_3(T) = \frac{C_2^2}{C_1^4} - \frac{2 \, C_3}{C_1^3} = \left[4^{-\frac{d}{\alpha}} - \tfrac{2}{3} \cdot 3^{-\frac{d}{\alpha}}\right] \lambda_T^{2d} \, .$$

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We have $\alpha = \frac{5}{2}$, so $\frac{d}{\alpha} = \frac{4}{5}$ for $d = 2$ and $\frac{6}{5}$ for $d = 3$.

(c) For photon statistics, the energy is

$$E(T,V) = V \int\limits_{-\infty}^{\infty} d\varepsilon \, g(\varepsilon) \, \varepsilon \, \frac{1}{e^{\varepsilon/k_{\mathrm{B}}T} - 1} = \frac{V \Omega_d \, \varepsilon_0}{(2\pi\ell)^d \, \alpha} \, \Gamma\!\left(\tfrac{d}{\alpha} + 1\right) \zeta\!\left(\tfrac{d}{\alpha} + 1\right) \left(\frac{k_{\mathrm{B}}T}{\varepsilon_0}\right)^{\frac{d}{\alpha}+1}$$

Thus,

$$C_V = \frac{\partial E}{\partial T} = \frac{V \Omega_d \, k_{\mathrm{B}}}{(2\pi\ell)^d \, \alpha} \, \Gamma\!\left(\tfrac{d}{\alpha} + 2\right) \zeta\!\left(\tfrac{d}{\alpha} + 1\right) \left(\frac{k_{\mathrm{B}}T}{\varepsilon_0}\right)^{\frac{d}{\alpha}} .$$

($\mathbf{3}$) At atmospheric pressure, what would the temperature T have to be in order that the electromagnetic energy density should be identical to the energy density of a monatomic ideal gas?

Solution :

The pressure is $p = 1.0\,\mathrm{atm} \simeq 10^5\,\mathrm{Pa}$. We set

$$\frac{E}{V} = \tfrac{3}{2} \, p = \frac{2\pi^2}{30} \, \frac{(k_{\mathrm{B}}T)^4}{(\hbar c)^3} ,$$

and solve for T:

$$T = \frac{1}{1.38 \times 10^{-23}\,\mathrm{J/K}} \cdot \left[\frac{45}{2\pi^2} \cdot (10^5\,\mathrm{Pa}) \cdot \left(1970\,\mathrm{eV\,\mathring{A}} \cdot 1.602 \times 10^{-19}\,\frac{\mathrm{J}}{\mathrm{eV}} \cdot 10^{-10}\,\frac{\mathrm{m}}{\mathring{A}}\right)^3\right]^{1/4}$$

$$= 1.19 \times 10^5\,\mathrm{K} .$$

(4) Consider a two-dimensional gas of fermions which obey the dispersion relation

$$\varepsilon(\mathbf{k}) = \varepsilon_0 \left((k_x^2 + k_y^2)\,a^2 + \tfrac{1}{2}(k_x^4 + k_y^4)\,a^4\right) .$$

Sketch, on the same plot, the Fermi surfaces for $\varepsilon_{\mathrm{F}} = 0.1\,\varepsilon_0$, $\varepsilon_{\mathrm{F}} = \varepsilon_0$, and $\varepsilon_{\mathrm{F}} = 10\,\varepsilon_0$.

Solution :

It is convenient to adimensionalize, writing

$$x \equiv k_x a \quad , \quad y \equiv k_y a \quad , \quad \nu \equiv \frac{\varepsilon}{\varepsilon_0} . \tag{1}$$

Then the equation for the Fermi surface becomes

$$x^2 + y^2 + \tfrac{1}{2}x^4 + \tfrac{1}{2}y^4 = \nu . \tag{2}$$

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In other words, we are interested in the *level sets* of the function $\nu(x, y) \equiv x^2 + y^2 + \frac{1}{2}x^4 + \frac{1}{2}y^4$. When ν is small, we can ignore the quartic terms, and we have an isotropic dispersion, with $\nu = x^2 + y^2$. *I.e.* we can write $x = \nu^{1/2}\cos\theta$ and $y = \nu^{1/2}\sin\theta$. The quartic terms give a contribution of order ν^4, which is vanishingly small compared with the quadratic term in the $\nu \to 0$ limit. When $\nu \sim \mathcal{O}(1)$, the quadratic and quartic terms in the dispersion are of the same order of magnitude, and the continuous $O(2)$ symmetry, namely the symmetry under rotation by any angle, is replaced by a discrete symmetry group, which is the group of the square, known as C_{4v} in group theory parlance. This group has eight elements:

$$\{\mathbb{I}, R, R^2, R^3, \sigma, \sigma R, \sigma R^2, \sigma R^3\} \tag{3}$$

Here R is the operation of counterclockwise rotation by $90°$, sending (x, y) to $(-y, x)$, and σ is reflection in the y-axis, which sends (x, y) to $(-x, y)$. One can check that the function $\nu(x, y)$ is invariant under any of these eight operations from C_{4v}.

Explicitly, we can set $y = 0$ and solve the resulting quadratic equation in x^2 to obtain the maximum value of x, which we call $a(\nu)$. One finds

$$\tfrac{1}{2}x^4 + x^2 - \nu = 0 \qquad \Longrightarrow \qquad a = \sqrt{\sqrt{1 + 2\nu} - 1}. \tag{4}$$

So long as $x \in \{-a, a\}$, we can solve for $y(x)$:

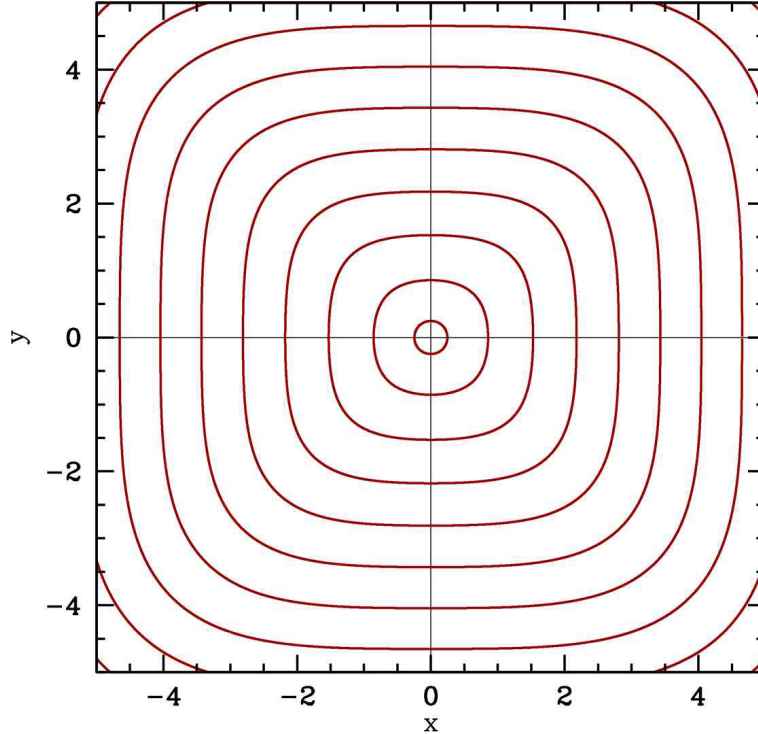$$y(x) = \pm\sqrt{\sqrt{1 + 2\nu - 2x^2 - x^4} - 1}. \tag{5}$$

Figure 1: Level sets of the function $\nu(x, y) = x^2 + y^2 + \frac{1}{2}x^4 + \frac{1}{2}y^4$ for $\nu = (\frac{1}{2}n)^4$, with positive integer n.

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A sketch of the level sets, showing the evolution from an isotropic (*i.e.* circular) Fermi surface at small ν, to surfaces with discrete symmetries, is shown in fig. 1.

(5) Consider a set of N noninteracting $S = \frac{1}{2}$ fermions in a one-dimensional harmonic oscillator potential. The oscillator frequency is ω. For $k_{\mathrm{B}}T \ll \hbar\omega$, find the lowest order nontrivial contribution to the heat capacity $C(T)$, using the ordinary canonical ensemble. The calculation depends on whether N is even or odd, so be careful! Then repeat your calculation for $S = \frac{3}{2}$.

Solution :

The partition function is given by

$$Z = g_0 \, e^{-\beta E_0} + g_1 \, E^{-\beta E_1} + \dots \,,$$

where g_j and E_j are the degeneracy and energy of the jth energy level, respectively. From this, we have

$$F = -k_{\mathrm{B}}T \ln Z = E_0 - k_{\mathrm{B}}T \ln\!\big(g_0 + g_1 \, e^{-\Delta_1/k_{\mathrm{B}}T} + \dots\big) \,,$$

where $\Delta_j \equiv E_j - E_0$ is the excitation energy for energy level $j > 1$. Suppose that the spacings between consecutive energy levels are much larger than the temperature, *i.e.* $E_{j+1} - E_j \gg k_{\mathrm{B}}T$. This is the case for any harmonic oscillator system so long as $\hbar\omega \gg k_{\mathrm{B}}T$, where ω is the oscillator frequency. We then have

$$F = E_0 - k_{\mathrm{B}}T \ln g_0 - \frac{g_1}{g_0} \, k_{\mathrm{B}}T \, e^{-\Delta_1/k_{\mathrm{B}}T} + \dots$$

The entropy is

$$S = -\frac{\partial F}{\partial T} = \ln g_0 + \frac{g_1}{g_0} \, e^{-\Delta_1/k_{\mathrm{B}}T} + \frac{g_1}{g_0} \, \frac{\Delta_1}{T} \, e^{-\Delta_1/k_{\mathrm{B}}T} + \dots$$

and thus the heat capacity is

$$C(T) = T \frac{\partial S}{\partial T} = \frac{g_1}{g_0} \, \frac{\Delta_1^2}{k_{\mathrm{B}}T^2} \, e^{-\Delta_1/k_{\mathrm{B}}T} + \dots$$

With $g_0 = g_1 = 1$, this recovers what we found in §4.10.6 of the Lecture Notes for the low temperature behavior of the Schottky two level system.

OK, so now let us consider the problem at hand, which is the one-dimensional harmonic oscillator, whose energy levels lie at $E_j = (j + \frac{1}{2})\hbar\omega$, hence $\Delta_j = j\hbar\omega$ is the jth excitation energy. For $S = \frac{1}{2}$, each level is twofold degenerate. When N is even, the ground state is unique, and we occupy states $|\, j\,,\uparrow\,\rangle$ and $|\, j\,,\downarrow\,\rangle$ for $j \in \{0\,,\,\dots\,,\,\frac{N}{2}-1\}$. Thus, the ground state is nondegenerate and $g_0 = 1$. The lowest energy excited states are then made, at fixed total particle number N, by promoting either of the $|\, j = \frac{N}{2}-1\,,\,\sigma\,\rangle$ levels ($\sigma = \uparrow$ or $\downarrow$) to $|\, j = \frac{N}{2}\,,\,\sigma'\,\rangle$. Accounting for the possibility of spin flips, there are $g_1 = 4$ ways to do this,
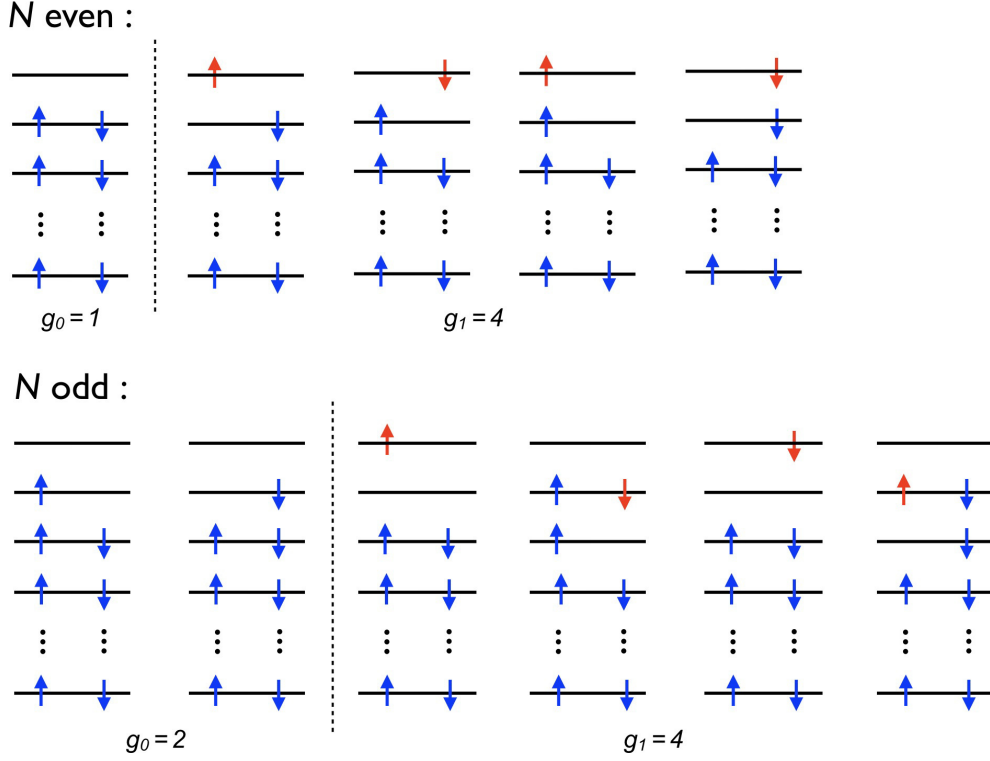
Figure 2: Ground states and first excited states for the $S = \frac{1}{2}$ one-dimensional simple harmonic oscillator.

each of which increases the energy by $\Delta_1 = \hbar\omega$ (see Fig. 2). When N is odd, we fill one of the spin species up to level $j = \frac{N-1}{2}$ and the other up to level $j = \frac{N+1}{2}$. In this case $g_0 = 2$. What about the excited states? It turns out that $g_1 = 4$, as can be seen from the diagrams in Fig. 2. For N odd, in either of the two ground states, the highest occupied oscillator level is $j = \frac{N+1}{2}$, which is only half-occupied with one of the two spin species. To make an excited state, one can either *(i)* promote the occupied state to the next oscillator level $j = \frac{N+3}{2}$, or *(ii)* fill the unoccupied state by promoting the occupied state from the $j = \frac{N-1}{2}$ level. So $g_1 = 2 \cdot 2 = 4$. Thus, for either possibility regarding the parity of N, we have $g_1/g_0 = 2$, which means

$$N \text{ even}: \quad C(T) = \frac{4(\hbar\omega)^2}{k_B T^2} e^{-\hbar\omega/k_B T} + \ldots$$

$$N \text{ odd}: \quad C(T) = \frac{2(\hbar\omega)^2}{k_B T^2} e^{-\hbar\omega/k_B T} + \ldots$$

This result is valid for $N > 1$.

An exception occurs when $N = 1$, where the lone particle is in the $n = 0$ oscillator level. Since there is no $n = -1$ level, the excited state degeneracy is then $g_1 = 2$, and the heat capacity is half the above value. Of course, for $N = 0$ we have $C = 0$.

What happens for general spin S? Now each oscillator level has a $K \equiv 2S+1$ spin degen-
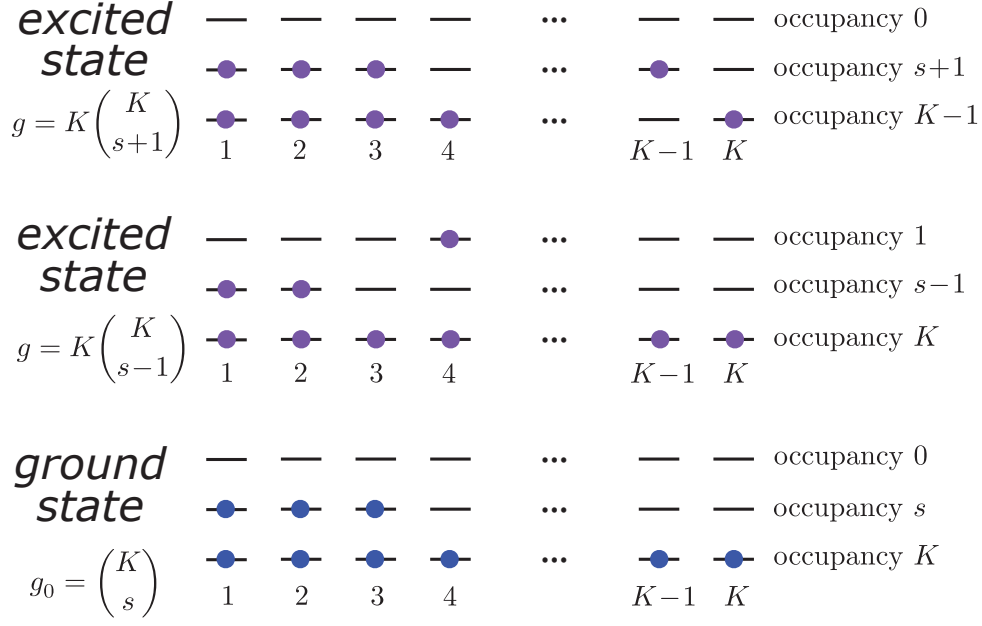
Figure 3: Ground states and first excited states for the general S case, with $K = 2S+1$.

eracy. We may write $N = rK + s$, where r and s are integers and $s \in \{0, 1, \ldots, K-1\}$. The ground states are formed by fully occupying all $|j, m\rangle$ states, with $m \in \{1, \ldots, K\}$, from $j = 0$ to $j = r-1$. The remaining s particles must all be placed in the K degenerate levels at $j = r$, and there are $\binom{K}{s}$ ways of achieving this. Thus, $g_0 = \binom{K}{s}$.

Now consider the excited states. We first assume $r > 0$. There are then two ways to make an excited state. If $s > 0$, we can promote one of the s occupied states with $j = r$ to the next oscillator level $j = r+1$. One then has $s-1$ of the K states with $j = r$ occupied, and one of the K states with $j = r+1$ occupied. The degeneracy for this configuration is $g = \binom{K}{1}\binom{K}{s-1} = K\binom{K}{s-1}$. Another possibility is to promote one of the filled $j = r-1$ levels to the $j = r$ level, resulting in $K - 1$ occupied states with $j = r-1$ and $s+1$ occupied states with $j = r$. This is possible for any allowed value of s. The degeneracy of this configuration is $g = \binom{K}{K-1}\binom{K}{s+1} = K\binom{K}{s+1}$. Thus,

$$g_1 = K\binom{K}{s+1} + K\binom{K}{s-1},$$

and thus for $r > 0$ and $s > 0$ we have

$$C(T) = \frac{g_1}{g_0} k_{\mathrm{B}} \left(\frac{\hbar\omega}{k_{\mathrm{B}}T}\right)^2 e^{-\hbar\omega/k_{\mathrm{B}}T} + \ldots$$

$$= K \cdot \left\{ \frac{K-s}{s+1} + \frac{s}{K-s+1} \right\} \cdot k_{\mathrm{B}} \left(\frac{\hbar\omega}{k_{\mathrm{B}}T}\right)^2 e^{-\hbar\omega/k_{\mathrm{B}}T} + \ldots$$

The situation is depicted in Fig. 3. Upon reflection, it becomes clear that this expression

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is also valid for $s = 0$, since the second term in the curly brackets in the above equation, which should be absent, yields zero anyway.

The exceptional cases occur when $r = 0$, in which case there is no $j = r - 1$ level to depopulate. In this case, $g_1 = K\binom{K}{s-1}$ and $g_1/g_0 = Ks/(K-s+1)$. Note that all our results are consistent with the $K = 2$ case studied earlier.