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Anatomy of Thermodynamics of Open Shell and Finite Volume.

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Abstract : For fermions, the chemical potential cannot be less than the single particle ground state energy since it leads to negative specific heat ! In other words to do thermodynamics of open shell systems, one cannot take the Fermi distribution function to be a fraction. Finite volume calculations are sometimes done using continuum states. This is questionable as such but also leads to artificial "volumes" when open shell problems are encountered.

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It is well known that a fermion, with energy levels q_i in a single particle Hamiltonian, put in thermal bath at temperature T, the number at equilibrium is :

$$N_{\pm} = \sum_i G_i f_{\pm}, \tag{1}$$

where G_i are the degeneracy factors of the levels and the Fermi-function f_i is given for particles (+, antiparticles -) by :.

$$f_i(\pm) = 1/(1 + \exp \frac{q_i \pm \mu}{T}). \tag{2}$$

Here μ is the chemical potential which is found by fixing the number given in eq.(1).

When one has the problem of putting 3 quarks in a state with degeneracy 12, or two nucleons is the s-d shell of the nuclear model with degeneracy 12, at zero temperature, one is tempted to use f_0 which is 1/4 or 1/6 respectively by making μ less than the ground state energy, q_0. But the entropy is given by [1] :

$$S(\pm) = -\sum_i [f_i(\pm) ln(f_i(\pm)) + (1 - f_i(\pm))ln(1 - f_i(\pm))]G_i \tag{3}$$

and this prescription leads to a positive non-zero entropy for the system at zero temperature. The purpose of the present paper is to show that this is wrong. The energy of the particles (antiparticles) in the system are given by

$$E(\pm) = \sum_i q_i G_i f_i(\pm) \tag{4}$$

One can define the free energy of the system which is

$$F \equiv E - TS \tag{5}$$

where the energy and the entropy are summed over particles and antiparticles. For systems where the number is kept constant, using the second law we get :

$$S = -(\partial F/\partial T)_V \tag{6}$$

The specific heat is given by :

$$C_V \equiv (\partial E/\partial T)_V. \tag{7}$$

For T = 0, $F = E$, so that from eq.(6) and eq.(7), we get $S = -C_V$, the specific heat at constant volume. Positive non-zero entropy at zero T thus implies a negative specific heat. This may be the origin of the mysterious negative C_V, encountered in nuclear physics calculations of [2], who state that this means the solution is thermodynamically

unstable[1]. It is not clear then how these solutions, which have a wrong low T behaviour can still be used at high T. Even in particle physics [4] one can associate degrees of freedom with C_V and negative degrees of freedom is also absurd. However, if $\mu \geq e_0$, f_0 is one for the ground state and zero for other states, the entropy and C_V goes to zero at T = 0 and there is no contradiction. In this case one has to drop the multiplicity factors and fix the number in eq.(1) to be one and multiply the energy and the entropy by the actual number of particles. The requirement that number $N > G_i$, needed for derivation of quantum statistics [1] is just about satisfied in this case !

It is interesting to consider the case of the thermodynamic limit, in which case the energies are continuous and start from zero. In this case the sum in eq.(1) is replaced by an integration over the continuous q, with a $(V/(2\pi^3)$ factor. So now the condition $\mu > q_0$, is replaced by μ positive, and eq.(1) is always satisfied at the expense of parametrizing the volume V. But the volume is infinite, and so one does not consider number, but number density, and in this way the cutoff in q, called the Fermi momentum is fixed by the degeneracy g which replaces G_i. For neutron star matter therefore the density to Fermi momentum ratio is not the same as for nuclear matter, there being the extra isospin degeneracy in the latter case. Sometimes in quark physics, without taking the volume infinite, one still approximates the discrete states by energies that are continuous and start from zero [5], [6], [7]. Now the volume is fixed by eq.(1). These volumes are once again mysterious, not the physical volumes. They are found to be artificially large. For example Mac and Ugaz [5], find the radius of the nucleon to be larger than 2 fm, so that the volume is more than ten times the experimental one, which prompts them to comment that their parton distributions "could be appropriate for larger systems such as heavy nuclei, hesvy-ion collisions or even in the early Universe". Another mystery that appears when one tries to colour projection with these continuum states, one needs imaginary chemical potential [8] ! This is to avoid infinities in summing over group parameters and is not necessary when one is doing calculations with discrete states [9].

The importance of finite size was stressed in [10]. Recently it has been emphasized again in the context of heavy ion (HI) physics [11]. Using the bag model we have succesfully calculated the density of states of mesons [12] and compared with string theory [13]and experiment. Extension for baryons has also been done [14].

To summarize we have suggested that use of fractional occupation number for open shell problems may lead to "unsavoury" objects like negative specific heat and positive entropy at zero T. Use of continuous states with finite volume leads to problems also. With finite volume and discrete states one can calculate effects in heavy ion and density of states in particle physics.

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[1]see also [3]

doctorate) S. N. Bose, who started quantum statistics 70 years back and whose centenary we are celebrating this year.

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