**Generalized Statistical Mechanics and the Partition Function**

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In previous notes, we argued one may find the number of particles in a state ei by using time reversal elastic two body scattering balance. This approach yields the Maxwell-Boltzmann (MB), Fermi-Dirac (FD) and Bose-Einstein (BE) distributions and has also been applied to more generalized cases. The approach makes no use of entropy or partition functions and seems to be very close to that used by Kaniadakis (1), although he develops a Fokker-Planck equation and defines an entropy. His entropy, however, seems to be a mathematical construct, created by integrating a function of f so that one may later take the derivative with respect to f and obtain the original function. This original function is then equated to -(e-u)/T (u=chemical potential) from a Lagranian multiplier. It seems, however, that if an entropy is defined, one may calculate a Free Energy and try to link this to a canonical (or grand canonical partition function). In (2), a different generalized theory of statistical mechanics is proposed. It too calculates entropy density, but obtains a different functional form. Imposing the “scattering constraint” which both (1) and (2) ultimately seem to use, leads to similar results. In (2), however, a canonical and then grand canonical partition function is developed from the entropy. This seems to lead to different distributions than those predicted by the scattering approach. The objective is this note is to try to analyze these different theories to see why they appear to be different.

**Time Reversal Elastic Two Body Scattering Balance**

For the MB case, it is assumed the probability for e1 and e2 to collide is f(e1)f(e2). Thus for e1+e2=e3+e4 ((1a)), one has f(e1)f(e2)=f(e3)f(e4) ((1b)) for the probabilities of the forward and time reversed reactions to be equal. Taking ln of the latter and equating to energy conservation equation yields the MB distribution. It should be noted this distribution would be unnormalized i.e.:

ln(f(ei)) = -ei/T ((1))

Alternatively, one may write:

ln(f(ei))= - (ei-u)/T ((2)) u plays the role of a chemical potential, but is also part of the normalization constant.

For the FD or BE case, it has been argued in previous notes, one may generalize ((1b)), but leave ((1a)) alone. This accounts for restrictions or enhancements due to fermion or boson scattering. Thus:

ln( f(ei) / [1-/+ f(ei)] ) = -(ei-u)/T ((3)) - for fermions + for bosons.

Here f(ei) is not normalized to 1, but rather to N, the total number of particles. Given that u appears, it seems one is “using” the grand canonical philosophy.

For a more generalized reaction, one may have g(f(ei),ei) replace f(ei) in ((1b)). Then ((3)) becomes:

ln( g(ei) / [1-/+ f(ei)] ) = -(ei-u)/T   ((4))    - for fermions  + for bosons.

There is no appearance of an entropy or partition function in the scattering approach and it seems to be directly linked to the physics of the problem and not so much to statistics.

If one examines ((4)), one may notice it is in the form of:

ln(k(f(ei)) = -(ei-u)/T   ((5))

In fact, Kaniadakis (1) argues this is the most general result from kinematics. He, however, does not solve for f(ei) equilibrium from ((5)) directly, but establishes a Fokker-Planck equation and an entropy density which finally yields the same result as ((5)).

In (1), he does not take the entropy density and calculate a free energy which one may then link to a canonical or grand canonical partition function as is done in (2).

**Calculation of Kaniadakis Entropy and Other Entropies**

Kaniadakis defines entropy density as:

Sd = - Integral df  ln(k(af(ei)) )    ((6))   Here we set a=1

Entropy =  S= Integral  d phase space    Sd   ((7))

Given ((5)), however, ((6)) is equivalent to:    f (ei-u)/T  ((8))  so entropy is

S= Eave - uN/T   ((9))

((6)) is general, which allows it to be used in a “maximization” approach with two constraints, one for average energy and one for average particle number.

In (2), one does not use the “grand canonical philosophy” immediately. Rather, a grand canonical partition function is ultimately developed. Entropy is defined as:

-Integral dphase space f ln(k(f(ei)) , but with   ln(k(f(ei))= -ei/T.

Consider applying ((6)) to the fermion example of ((3)). Then:

Sd= - Integral df ln[f/(1-f)] = - f ln(f) +f - (1-f) ln(1-f) + (1-f) ((9))

Integrating over phase space yields:

S= {Integral dphase space -ln[ f/(1-f)] } + (N+1-N) - Integral dphase space ln(1-f)

Using ((5)) yields: S= Eave/T - uN/T+ (N+1-N) - Integral dphase space ln(1-f) ((10))

For the FD distribution, it is known that f(e) = 1/ [1+ exp( (e-u)/T) ]. Thus:

Integral dphase space ln(1-f) = Integral dphase space ln[1+exp(-1/T(e-u))}

This makes Kaniadakis entropy identical (except for the +T term) to the FD entropy given in textbooks i.e. (3):

S(FD) = Sum over gi { {(1/T) ei - ln(z)} / {$z^{-1}$ exp(1/T(e)+1} + ln(1+z exp(-ei/T)) }

Here z=exp(u/T) and Sum over gi = Integral d phase space.

For ((11))

It should be noted in ((5)) that if one uses (ei-u)/T, one is already thinking in terms of the grand canonical approach and therefore cannot sum over n states a second time.
If one treats u/T and 1/T as independent variables, one may try to find average energy by using: d (F/T) / d(1/T) and the particle number from d(F/T) / du applied essentially to Integral dphase space ln(1-f). One sees this yields the average energy and particle number so there is a grand partition partition function. One does not need to extend it and sum over occupations 0 and 1.

In (2), S= Integral dphase space f $G^{-1}$(f) where $G^{-1}$ is ln(k). It is stated that TS = Eave - T ln (A) where A is the normalization of f(ei). This does not seem to follow directly from the definition in (2) unless one forces this -Tln(A) as a constant of integration. It is this constant of integration, however, which becomes F and is critical in the development of the canonical potential. Later, e is replaced with (e-u)ni.

A= integral dphase space f(ei) ((11b))

In (2), F=-kT ln(A) where A is the normalization of the generalized f. F is equated with the canonical partition function -kT lnZ.

Thus, in (2), the canonical partition function is given by:

Z= Integral dphase space f(e)

Next, (2) generalizes to a grand canonical partition function X where:

X = -kT ln{ Sum over ni Integral dphase space f( (ei-u)ni) } ((12))

where ni represents the range of allowed particle numbers for state ei. For example, for fermions, ni=0 or ni=1. In the next section, we try to compare the consequences of ((12)) with the time reversal scattering theory.

For the usual MB case, one defines a grand canonical partition function using:
X= Sum over N exp(Nu/T) Z(N) where Z(N) is the canonical partition function for N particles. The MB partition function makes use of exp(-E/T)= exp(- Sum over i eini/T), so u becomes associated with ei in the following manner: (ei-u)/T. In (2), the authors argue that if one has:

f=A(1+e/T)$^{-k-r}$ and dS/dN = -u/T then f should change to A(1+(e(N)-uN)/T)$^{-k-r}$.
(See equation ((15)) in (2).)

It seems the result of (2) is linked to G$^{-1}$(f) = -N/T (e-u). Thus, f=G(-N/T(e-u)).
This is similar to the scattering approach and Kaniadakis' approach except that those two do not use N, only (e-u). Thus, there is no extra summation over N as in (2). To see how this arrives in (2) in more detail, consider:

f(ei)= Integral de delta(ei+e-E) G[S(e) - S(E)]

As a first step, consider only a change in energy: S(e) approx = S(E) + 1/T (e-E). Then:
f(e) is proportional to G( (e-E)/T). For the case of variable E and N, one may expand:

S(e) approx = S(E) +1/T(e-E) + u/TN Then f(ei) is proportional to G( (e(N)-uN)/T ).
This is very similar to what is done for the scattering and Kaniadakis entropy except for those cases, there is no further sum over N and one uses f((ei-u)/T). The Kaniadakis entropy is already associated with a grand canonical partition function.

Thus, it seems that the time reversal elastic scattering balance differs in two ways from the approach of (2):

1) $S= E/T - T\ln(A)$ where A is the normalization of f(e) in (2). $S=E/T$ + constant where the constant may not be $T\ln(A)$ in the time reversal balance approach. It is $T\ln(A)$ for the MB case.
2) The approach of (2), changes f(e) to f((e(N)-uN)/T) for variable N and forces a grand canonical summing over states i.e. N=0 or 1 for a fermion. For the scattering approach, 1-f(e) is used to describe the restriction of scattering into a state e. For the MB case, the scattering approach is identical to the grand canonical partition function calculation, but it does not seem to hold for more general cases.

It seems the approach to handling entropy differs in the two cases. For the scattering case, one may use Kaniadakis entropy (1). For the MB fermion case, one has for entropy:

Integral dphase space F ln(f) - (1-f)ln(1-f) - f +(1-f). The last two terms are not important.
This, as shown yields, Eave/T - u/TN + integral dphase space ln(1-f) where the integral is:
Integral dphase space [1+exp(-1/T (e-u))]. This is exactly the factor that emerges from a grand canonical partition function approach, namely:

Ln{ [0 + 1 exp(-1/T(e-u))] / [ 1+ exp(-1/T(e-u))]}

Thus, the restriction from scattering into occupied states lowers the entropy. Consider the more general case: ln(g(f)/(1-f))= -(e-u)/T. This leads to a Kaniadakis entropy of:

S=Integral dphase space Integral df ln(g(f)) - (1-f)ln(1-f) = Eave/T -uN/T - ln(1-f)

Thus, F= uN +Tln(1-f). The second term again represents a reduction due to the restriction of scattering into an occupied state, but does not seem to be easily obtainable by summing over 0 and 1 in a grand canonical scheme.

**Differences between the Time Reversal Balance and Generalized Grand Canonical Approaches**

For the time reversal balance approach, one has from ((4)) the generalized fermion result:

ln( g(f(ei)) / [1- f(ei)] ) = -(ei-u)/T ((14))

One needs to know g as a function of f and then may solve for f(ei).
Consider, as in (2), the following:

$f(e) = (1+ e/k)^{-k-r}$ (this is without the incorporated fermion effects) and $G^{-1}(f) = (f^{-1/(k+r)} - 1)\, k$ ((15))

In the scattering picture, one uses: $G^{-1}(f) / (1-f) = -(ei-u)/T$ the factor 1/(1-f) represents the fact that a fermion may not scatter into a state that is occupied.

Let v=(-(ei-u)/T) and k+r= 1, then (1/f-1)k = (1-f)v ((16))

((16)) may be solved as a quadratic:

f (FD) = ni(FD) = $\{(v+k) +/- \mathrm{sqrt}((v+k)^2 -4vk) \} / 2v$ ((17)) (ni is the number of particles in state ei)

If one uses the approach of (2),on finds the following for ni(FD):

W= - Tln {G(ni=0) +G(ni=1)} where $G=(1+ ni(ei-u)/k)^{-k-r}$

For k+r=1 ni (FD) = d/du W = Constant / [ G(0) + G(1) ] = 1/[ 2+ (e-u)/T] ((17))

((16)) and ((17)) do not appear to be the same. Thus, there seems to be a difference in the time reversal elastic scattering balance approach and the generalized statistical mechanical approach of (2).

**Conclusion**

In conclusion, in previous notes we have tried to present a time reversal elastic two body scattering balance equation as a method for obtaining distributions. Such an approach does not make use of entropy or partition functions. In the literature, however, it seems use is made of both. In (1), an entropy is developed, but it seems to be created by integrating a function over df (so that later it may differentiated by d/df). Nevertheless, this entropy for the fermion case matches that of statistical mechanical textbooks (3). No partition function approach is developed. In (2), an entropy is developed, but it seems an integration constant -kTln(A) where A is the normalization of f(e) enters in a possibly unusual manner. This is critical as -kTln(A) becomes the free energy which is equivalent to the canonical partition function. The canonical partition function is then converted into a grand canonical partition function by replacing ei with (ei-u)ni and ni summed over allowable states. This approach also seems to differ from statistical mechanical texts where Grand canonical partition = Sum over N exp(u/T) Q(N) where Q(N) is the canonical partition function for N particles. For example for the Fermi-Dirac case, it would be summed over ni=0 and ni=1. This leads to a generalized Fermi-Dirac distribution which does not seem to agree with that obtained by using the time reversal elastic scattering balance approach.

References

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