Reactions, Distributions and Entropy in Generalized Statistical Mechanics

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For a number of years, articles have appeared in the literature describing statistical mechanics which goes beyond that of the Boltzmann-Gibbs-Shannon picture (1),(2),(3). In addition, it seems two particular entropy density Sd functional forms in terms of the distribution f((e-u)/T), where u is the chemical potential, appear frequently. The first is Sd=- f ln(g(f)) and the second, Kaniadakis (1) Sd = - Integral df ln(g(f)) where ln(g(f)) = -(e-u)/T. In this note, we argue first that one is not abandoning Shannon's entropy in general statistical mechanics, but rather is applying it to the number of reactions of a particle with energy ei, rather than to particle number. Thus, Shannon's entropy is - g ln(g). This entropy, however, applies to reactions, not particles. Secondly, we try to show that it is Kaniadakis form of the particle entropy which is consistent with both thermodynamics and the Jaynes idea of maximizing particle entropy to find the distribution function.

Time Reversal Balanced Elastic Scattering

We have argued in a number of previous notes that one may obtain particle distributions by utilizing a time reversal elastic two body scattering approach which does not make use of counting(factorials), entropy or partition functions. In particular, one tries to find an independent scattering probability, namely:

ln(g(f((ei-u)/T)) = - (ei-u)/T where u is the chemical potential and e1+e2=e3+e4 ((1))

For the Maxwell-Boltzmann, case g is the identity function, for the Fermi-Dirac case g=f/(1-f) and for the Bose-Einstein case g=f/(1+f). Other g functions pertain to other more generalized situations.

One may note from ((1)), however, that g(f)= exp(-(e-u)/T. This is the Maxwell-Boltzmann form, but it applies to the scattering probability g, not the particle number probability f. Thus, scattering follows Shannon's entropy we argue. In particular, one may use the usual statistical mechanical approach of maximizing:

M! / (m1! m2! …..) subject to the constraint Sum over i mi ei = MX ((2))

Here mi is the number of reactions involving a particle with energy ei and X is not the average energy. (Note: Sum over i f((ei-u)/T) ei = MU where U is the average energy still exists.) Following (4), ((2)) is generalized to the complex plane and a saddle point approach used. This leads to a probability of the form exp(Shannon's entropy) and then to the canonical partition weight exp(-E/T). Thus, counting(factorials), Shanon's entropy, the maximization of entropy and the canonical partition function are all linked. For regular statistical mechanics, g=the identity function, so f(ei) is both the probability for a particle with energy ei to scatter and it is the particle distribution as well. For the more general case, the two are not the same. Thus, Shannon's approach seems to apply to scattering, not to the particle distribution function. The latter may be obtained from ((1)).

Thus, we suggest Shannon's entropy density holds for scattering, namely

Sd scattering = $- g(f) \ln(g(f))$ ((3))

Entropy Considerations

Although ((3)) is a scattering entropy density, it is the particle entropy which is needed for thermodynamics. Thus, one needs to determine its form. In the literature, two approaches seem to be used. In (3) and (5), the following form seems to appear:

Sd = $-(ei-u)/T\ f(ei)$ ((4))

When integrated, this leads to Eave - uNave ((4))

Kaniadakis (1), however, defines a different density, namely:

Sd = Integral df g(f) ((5))

((5)) is developed so that:

d/df Sd - d/df (e-u)/T f = 0 ((6)) Thus, a Jaynes type of maximization of entropy density applies. In other words, one integrates over df in ((5)) so that the inverse operation d/df returns ln(g) which from ((1)) equals (e-u)/T. In the case of ((6)) (e-u)/T is brought in as a Lagrange multiplier. An interesting feature of the Kaniadakis entropy is that it is consistent with Fermi-Dirac and Bose-Einstein entropies calculated from counting methods in traditional statistical mechanics (4). The Kaniadakis entropy may then be used to obtain the grand canonical partition function.

Determining an Entropy Consistent with Jaynes Maximization and Thermodynamics

Consider trying to find an entropy density Sd as a function of f which is consistent with both thermodynamics and Jaynes' approach of maximizing entropy by varying f.

In thermodynamics, consider TSd= Ed(f) + B(f) ((7)). Here Ed(f) is the average energy minus uN given by f (e-u)/T. We use the form of ((7)) so that B(f) becomes the free energy F=E-TS+uN.

Then: TSd = f ln(g(f)) + B(f). ((8))

Using ((8)) as the Jaynes entropy to be maximized subject to the Lagrange multiplier (e-u)/T yields:

d/df {- f ln(g) +B(f) - (e-u)/T f) = 0 or ln(g)=(e-u)/T ((9a)) and - f d/df [ln(g)] + dB/df = 0 ((9b))

Thus, one must solve ((9b)), but this yields, using integration by parts on f d [ln(g)]:

f ln(g) - Integral df ln(g) = B ((10))

Thus, B- f ln(g) = - Integral df ln(g) which is Sd, the entropy density. Thus, one finds that Kaniadakis entropy -Integral df ln(g) is consistent with thermodynamics.

Conclusion

In conclusion, we argue one may obtain particle number distribution functions f((e-u)/T) by applying Shannon's entropy ideas to "scattering" and not to particle number probability. In other words: ln(g(f))= -(e-u)/T. One does not need entropy, counting or partition functions to find f(ei). Nevertheless, for independent scattering, the scattering follows the ideas of factorial counting, Shannon's entropy and the idea of the canonical partition function, although exp(-E/T) is not the weight. Thus, we argue -g(f) ln(g(f)) is Shannon's entropy for scattering. (In the Maxwell-Boltzmann case, g=identity and so the Shannon's entropy describes both the scattering entropy and the particle number entropy at the same time.)

In thermodynamics, however, one is not interested in a scattering entropy, one needs particle number entropy. In this note, we try to show that such a thermodynamic entropy, consistent with Jaynes maximization of entropy density, subject to the Lagrange multiplier 1/T (e-u), leads to Kaniadakis entropy - Integral df ln(g(f)).

References

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