Oscillator Semiclassical Phase Space Probability versus a Quantum Mechanical Approach

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The Maxwell-Boltzmann probability factor exp(-energy/T) / normalization may be applied to a quantum oscillator using energy levels given by hbar w (n+.5). This leads to the derivative in 1/T of a geometric series and yields an average energy: Eave = hbar w/2 + hbar w / (-1+exp(hbar w/T)).

If one were to consider a semiclassical approach using p (momentum and x), energy would be described by pp/2 + xx/2 where for simplicity m=1 and k=1. This would appear in the MB factor with a temperature T and this expression would be expected to hold for high T or w/T small i.e. the quantum phonon jumps would be hardly noticeable compared to the average energy T in this limit.

If one tries to write the classical energy, for w/T small, in the form of quantum energy, one has hbar w n in this limit, where n is the number of phonons (hbarw/2 is small in this limit) so: zz= {pp/2+kk/2}/w is the number of phonons which should be multiplied by hbar w/T. One may then ask: What function has the limit hbar w/T? A solution is: {1-exp(-hbarw/T)}.

Thus the semiclassical normalized phase space probability: P(p,x) = {1-exp(-hbarw/T)}. Exp{ -zz {1-exp(-hbarw/T)} } yields the small hbar w/T limit quantum average energy. As a result, the average energy in this limit should match for both the classical phase space distribution and the quantum average energy expression. This classical distribution happens to be identical to the Husimi distribution.

One may note (as is done in (1)), that {1-exp(-hbarw/T)} is the probability for the quantum oscillator particle to be in the ground state. In the limit of hbar w/T small, this probability is hbar w/T which is a measure of the effect of the quantum phonon leaps as well. Fisher's information, as noted in (1), is equivalent to this ground state probability, but it is also the average energy which is proportional to the temperature type value, in this case {1-exp(-hbarw/T)}. This follows from the same kind of calculation done for a gas with particles with energy pp/2m, although instead of a factor of .5T one T because there is a contribution from pp/2 and xx/2.

Average Energy for a Quantum Oscillator

Using the Maxwell-Boltzmann form for probability(ei,T) =exp(-ei/T)/Z with ei = hbar w (n+.5) as single particle probability, one may calculate the average single particle energy as:

Eave = Sum over i hbar w (n+.5) exp(-ei/T)/Z = - d/d (1/T) ln(Z) ((1))

with Sum over i P(ei) =1. This condition gives, using the sum of a geometric series:

Z = exp(-hbar w/T) / { 1- exp(-hbarw/T) } ((2))

Using ((2)) for Z in ((1)) yields: Eave = hbar w/2 + hbar w / { -1 + exp(hbar w/T) } ((3))

Semiclassical Phase Space Approach

In classical physics, i.e. a phase space approach, one would still use an MB factor: exp(-ei/T)/Z, but energy would be given in terms of p and x i.e. for an oscillator:

p1p1/2m + kx1x1/2 = Energy ((4a))

Defining new p and x variables such that energy = pp/2 + xx/2, one may make use of the symmetry of x and p.

The MB factor t would be used in integrals over phase space i.e Integral dxdp / constant in one dimension. Given the symmetry of x and p:

Average energy:= Integral dp dx exp(-pp/2T) exp(-xx/2T) (pp/2 + xx/2)/ (ZZ) (hbar=1)

= 2/Z Integral dp exp(-pp/2T) pp/2 ((5)) (ZZ is the overall normalization)

= 2 { .5 kT) k=1 from the result for an average energy of a particle with only kinetic energy = .5mvv, or by performing the integral.

The semiclassical phase space approach should match the quantum result in the limit of high T or hbar w/T being very small. In this limit, the quantum energy:

E quantum = hbar w/2 + n hbar w ((6))

Thus exp(-Equantum/T) is approximately equal to: exp(- n hbar w/T) for n>>1. ((7))

One may try to cast the semiclassical distribution in the form of phonon energies i.e.:

-{pp/2 + xx/2} / w * w/T ((8))

Given that w/T only holds in the -hbar w/T very small limit, one may ask: What function reduces to w/T in this limit? A solution is:

[1- exp(-hbar w/T)] ((9))

Thus ((9)) becomes the 1/temperature type factor in the semiclassical normalized distribution:

P(x,p) semiclassical phase space = [1- exp(-hbar w/T)] exp{ -zz [1- exp(-hbar w/T)] } ((10))

Where zz = (pp/2 +xx/2)/(hbar w) as in (1).

The distribution ((10)) mimics the quantum probability weight in the hbar w/T very small limit.

It also happens to equal the Husima distribution.

What happens if one considers the opposite limit i.e. hbar w/T >>1. If T→0, this is satisfied and the particle should have a probability of 1 to be in the ground state. Small T values, however, also satisfy the condition. In such a case, quantum energy is:

Eave = hbar w/2 + hbar w / {exp(hbar w/T) - 1 } approx= hbar w/2

For the semiclassical distribution, average energy is proportional to hbar w * temperature like value i.e. hbar w /(1-exp(-hbarw/T)) approx equal to hbar w which is twice the quantum value because there is a contribution from pp and xx. Thus the semiclassical approach does not seem to work particularly well at low temperatures, but it is not expected to apply in such a region.

Husimi Distribution

Wigner developed a phase space probability function approximation for quantum wavefunctions given by (2):

f(p,x) = 1/h Integral dy exp(-ipy) W(x+y/2) W*(x-y/2) ((11))

where W(x) is the quantum wavefunction. f(p,x), however, may be negative which means that it is not an exact probability function.

((11)) is equivalent to: 1/h Integral dv W1*(p-.5v)W1(p+.5v) exp(ixq / hbar) ((12))

where W1(p) is the Fourier transform of the wavefunction W(x) i.e. the momentum wavefunction.

One may then create:

G(p,x) = 1/(3.14 hbar) Integral dv dy f(p+v,x+y) exp(-vv/ (2 dp dp)) exp(-yy/ (2 dx dx)) ((13))

If dp dx is set equal to hbar/2, ((13)) becomes the Husimi distribution:

Husimi(x,p) = 1/{ $(2*3.14)^{1.5}$ hbar dx} Modulus{ Integral (-infinite to infinite) dy W(y) exp(-ipy / hbar) exp(- (x-y)(x-y)/ (4 dx dx)) ((14))

The Husimi distribution is guaranteed to be positive within a certain range.

In (1), the Husimi distribution for a quantum oscillator is given as:

P(x,p) = (1-exp(-hbar w/T)) exp(- (1-exp(-hbar w/T)) xx) ((15))

where Mod Squared(z) = pp/(4aa) + xx/(4bb) where a= sqrt(hbar/2mw) and b= sqrt(hbar m w/2)

z= p/2a + i x/2b

In (1), a sum is performed over all eigenstates of the quantum oscillator i.e.

Husimi distribution = 1/Z Sum over n exp(-energy/T) <z|n> <n|z>   ((16))

with Z being a normalization and

<z|n> <n|z> = $|z|^2$/n! exp(- Mod Squared(z))   ((17))

Expression ((17)) = ((15)) represents the classical phase space distribution described at the beginning of this note.

Fisher Information

Fisher Information is a statistical quantity given for f(p,x) as:

Fisher Information = Integral dxdp f(p,x) { { d ln(f)/dx }{ d ln(f)/dx }+{ d ln(f)/dp }{ d ln(f)/dp } } ((18))

In (1) it is noted that Fisher Information using Husimi's distribution for a quantum oscillator is:

Fisher Information = (1-exp(-hbar w/T)   ((19))

This in turn is the probability for the oscillator to be in the ground state i.e.

Probability gs = exp(- hbar w/ (2T) / Z where Z = hbar w/2 / (1-exp(-hbar w/T) ((20))

This is not a surprise because Fisher Information is equivalent to average energy which is directly related to the standard deviation of the distribution (with <p>=<x>=0) i.e. the "temperature type parameter" of the Husimi distribution 1/(1-exp(-hbar w/T)). This holds because of the Gaussian forms of the results which also apply to a gas of particles with energy pp/2m. In this case, instead of average energy being proportional to .5T, it is proportional to T because of contributions from pp/2 and xx/2 which are identical.

Conclusion

In conclusion, we argue that if one consider the quantum oscillator results together with Maxwell-Boltzmann factor exp(- (quantum energy)/T) where energy = hbar w (n+.5), then in the non-quantum limit i.e. hbar w / T being very low, this MB factor should be similar to a semiclassical one: exp(- (pp/2 +xx/2) /T) where m and k are absorbed in p and x. To formally see the equivalence, one may write -(pp/2+xx/2)/T = -hbar w/T (pp/2+xx/2) / (hbar w) i.e. express the classical energy in terms of the number of phonons as done in the quantum case. This leaves the factor of - hbar w/T in the low hbar w/T limit. We then ask: What function becomes hbar w/T in this limit. The function (1-exp(-hbar w/T)) satisfies this criterion and yields the normalized semiclassical phase space distribution:

f(p,x) = (1-exp(-hbar w/T)) exp{ - (pp/2+xx/2)/(hbar w) (1-exp(-hbar w/T))}

It may be seen from the literature (1) that f(p,x) is equivalent to the Husimi distribution. Fisher information in this case is equivalent to average energy which is proportional to the "temperature type variable" in f(p,x) i.e. (1-exp(-hbar w/T). This in turn is the probability to be in the ground state.

References

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