Balance, Partition Function and Hamiltonians

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   Often, Lagrangians yielding the same equations of motion yield the same partition function. For the case of L= U(x)U(x) + mm/12 vvvv + mU(x) vv ((1)) this does not occur. As shown in (1), ((1)) yields the same same equations of motion as H = Hamiltonian = vv/2m + U(x) with p=mv, but the Hamiltonian of ((1)) is H= [vv/2m + U(x)][vv/2m + U(x)]. It is shown in (1), that the partition functions differ.

   In previous notes, we have argued that the partition function may be computed through two body scattering. In particular, the Maxwell-Boltzmann distribution follows from elastic scattering .5mv1v1 + .5mv2v2 = .5mv3v3 + .5mv4v4 and f(v1)f(v2) = f(v3)f(v4), where f(v) is the distribution function. We argue that one does not need a Hamiltonian to calculate a partition function, only a conserved quantity which does not change sign if $v \rightarrow -v$. In such a case, the two Hamiltonians yielding the same equations of motion need not be used in the partition function calculation. What matters, we argue, are the equations of motion which may be used to establish a conserved quantity. We argue that two body scattering defines the statistical system with any potentials accelerating the particle from one point to another. In some cases, a velocity dependent potential does not cause any acceleration. At a point of collision, one simply has velocities. At early points in x, one has kinetic energy plus any potential energy terms which cause acceleration and establish conservation of energy. Thus, the Hamiltonian of ((1)) yields the same equations as H=vv/2m + U(x) where p=mv, and U(x) is the potential which together with vv/2m ensures energy conservation. From this, one would calculate the usual partition function using vv/2m + U(x) as the conserved quantity.

Unusual Lagrangian

   We begin with the Lagrangian of (1)

L= -U(x)U(x) + mm/12 v⁴ + mU(x) vv   ((1))

The momentum is dL/dv = mm/3 vvv + 2mU v ((2)) and the Hamiltonian may be found from:

H= pv - L = [m/2 vv + U] [m/2 vv + U]   ((3))

This is the square of the usual Hamiltonian H1= m/2 vv + U(x). If m/2 vv + U(x) is a constant which it is because H is not a function of t, then H=H1H1 is also a constant.

To find the equations of motion, one may focus on v and x which are not the canonical variables x, p. Nevertheless, one obtains the physical equations of motion (following (1)).

First ((2)) yields: dv(p,x) / dp = 1/2m [1/ [U+vvm/2] ((4a)) and dv(x,p)/dx = -v dU/dx / [U + mvv/2] ((4b))

Then, one may calculate:

$dx/dt = dH/dp$ (x constant) $= dH/dv \, dv/dp = v$ ((5))   and

$dv/dt = dv/dx \, dx/dt + dv/dp \, dp/dt = -1/m \, dU/dx$ ((6))

((5)) and ((6)) are the usual results of H1= mvv/2 + U(x).

In (1), the partition function for the two Hamiltonians are calculated and found to differ. This may not be surprising because one Hamiltonian represents energy squared and not energy. Note: When using the Hamiltonian ((3)), the phase space is dp dx with p given by ((2)). One must convert to (.5mvv+U(x)) dx dv.

Scattering Balance

    We have argued in previous notes that one may calculate the Maxwell-Boltzmann factor using reaction balance for elastic scattering i.e.

$f(v1)f(v2) = f(v3)f(v4)$ ((7a))   where .5m v1v1 + .5m v2v2 = .5mv3v3 + .5m v4 v4   ((7b))

((7b)) is a conservation equation using a quantity,.5mvv, which does not change sign when v→ -v.

Taking the ln of ((7a)) and equating to ((7b)) yields the Maxwell-Boltzmann factor. No Hamiltonians are needed. The conservation law follows from the equations of motion. A collision occurs at a point x. To consider the distribution at other x points one may use conservation of energy .5mv(x)v(x) + U(x) = constant. Thus, the Maxwell-Boltzmann factor is: exp(- (.5mvv + U)/T) ((8)).
    We argue that two body scattering is the physical basis for the formation of equilibrium in classical statistical mechanics and potentials present may accelerate a particle from one point to another, but do not disrupt the equilibrium based on two body scattering. Only the density changes with x. T From the equation of motion one may find a conserved quantity i.e. E = .5mvv + U(x).

Alternatively, in standard statistical mechanics texts (2), it is argued that the number of states depends on energy i.e. not on energy squared etc.

Thus, there may be problems in using the Hamiltonian to establish a partition function if it does not represent energy.

Conclusion

In conclusion, we argue that although one may have different Hamiltonians yield the same equations of motion, but different partition functions, one may obtain the partition function weight from reaction balance. One only needs to find a conserved quantity involved with two particle scattering at a point x. This should be obtainable from the equation of motion, thus one does not need the explicit form of the Hamiltonian. The reaction balance is based on f(v1)f(v2) = f(v3)f(v3) with a conservation equation using a quantity which does not change sign as v→ -v.
This quantity is .5mvv which becomes .5mvv + U(x) when one considers that the particle changes energy from one point to another.

References

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2. Reif, F. Statistical and Thermal Mechanics (Wiley, 1986)