Operator Entropy and Quantum Thermodynamics

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The von Neumann entropy definition is -Tr (d ln(d)) and is linked to: <A> = Tr (d A) ((1)). Here d is a matrix as is A i.e Aij = <i A j>. As a result d is often not diagonal. It seems further that the idea of entropy is linked to an operator (2). In other words, one might have certain probabilities linked to the operator P momentum and a different set to X. For a diagonal d, von Neumann's form is the same as Shannon's entropy, but uses the eigenvalues of d.

For a pure quantum bound state Wn(x), it seems that one considers the two operators X and P and writes two entropies using Shannon's entropy form: - Integral dx W(x)W(x) ln(WW) and -Integral dp a(p)a(p) ln(a(p)a(p)) where W(x)=wavefunction= Sum over p a(p)exp(ipx). Here P(x)=W(x)W(x) and P(p)=a(p)a(p). For example in (3), one may see calculations of these "distinct" entropies for a particle in a box with infinite potential walls. X and P are linked to measurables and for a quantum bound system one cannot know exactly x and p at the same time.

One may write < KE > for a bound state in two ways:
Integral dp a(p)a(p) pp/2m or Integral dx W(x) (-1/2m d/dx dW/dx). Using Shannon's entropy approach one obtains two different entropy values Sx and Sp. With respect to von Neumann's entropy, it is zero for a pure state. Although one cannot know x and p at the same time (in terms of a measurement) that does not prevent one from writing x and p together (i.e. both known) in exp(ipx) for the wavefunction of a free particle. In this note we suggest that one might consider product probabilities linked to more than one operator when considering entropy. For example, for <KE> one may write Integral dx P(x) Integral dp pp/2m P(p/x) thus acknowledging that both x and p play a role. In this case, P(x)P(p/x) is the probability to use in Shannon's entropy as we have shown in (4). In (3) it is suggested that P(x)P(p/x) be used in order to incorporate both variables x and p. Using P(x)P(p) in Shannon's entropy yields the same overall entropy when integrated over x and p i.e. S=Sx+Sp.

One reason that the sum is useful is that it eliminates parameters such as L (box length) for a particle in a box with infinite walls (or k the spring constant for an oscillator. This allows for a quantum adiabatic transformation of a pure state to be isentropic. This follows from a Fourier transformation i.e. W(x)=Sum over p a(p)exp(ipx). The two variables p and x scale with L in the opposite manner i.e. x/L and pL (5). Thus we argue that entropy is not necessarily linked to only one operator, but rather for a pure state is linked to variables which appear in a Fourier transform. Usually a Fourier transform is simply a mathematical procedure, but not in the case of the quantum pure state wavefunction where the variable p is actually momentum.

In this note we try to investigate how the quantum relationship between p and x emerges. We argue that it exists at the level of the classical action for a free particle (relativistic or nonrelativistic) A=-Et+px where dA/dx partial =p and dA/dt partial = -E. Thus p and x are variable pairs in classical dynamics and this carries over to classical statistical phase space linked to p and x. We argue that a quantum dynamical link between p and x is also present in A i.e. -id/dx exp(iA) = p exp(iA). In other words p and x are linked dynamically in quantum mechanics as well (for a free particle) with exp(-iEt+ipx) being part of this link. The Fourier series form is already present in this solution as one may create a momentum distribution i.e.

Sum over p a(p)exp(ipx). This depends on p and x and both affect any operator based on p and x (or one of these). Thus we expect that probabilities linked to both p and x should appear in an expression of entropy for a quantum bound state.

Free Particle Dynamics and Quantum Bound States

Classical statistical mechanics characterizes particles based on x,p values which are part of Hamilton's equations. For example, one may write the classical free particle action (relativistic or nonrelativisic) as A=-Et+px and see that p and x are present. Furthermore: dA/dx partial = p and dA/dt partial =-E ((1)). Thus, single free particle dynamics are based on x and p. We argue that a quantum free particle is also based on x and p values i.e.

-id/dx partial exp(iA) = p exp(iA) and id/dt partial exp(iA) = Eexp(iA)   ((2))

In other words ((2)) represents eigenvalue equations linked to ((1)). X and p are as much part of the dynamics of a quantum system as of a classical. The complex probability objects exp(iA), however, make interpretation difficult as an ensemble of exp(ipx)'s interfere. From ((2)) one sees that exp(ipx) emerges without any notion of a Fourier series.
If one defines an ensemble of exp(ipx) values (dropping exp(-pp/2m t) factors because a new overall exp(-iEn t) term appears) one may define:

P(p/x) = a(p)exp(ipx)/W(x) where W(x) = Sum over p a(p)exp(ipx) = wavefunction ((3))

Thus exp(ipx) as part of a Fourier series emerges only in the definition of the x dependent normalization constant W(x). exp(ipx) is thus part of a probability which depends on x and p. Furthermore, scaling x→ x/L causes p→ pL if one wishes px to be unchanged. We have shown in (5) that one may obtain P(x)=W*(x)W(x) and P(p)=a*(p)a(p) from ((3)). These are classical type probabilities (i.e. real and positive) and are linked to observables, but do not describe the dynamics. It is W(x) and a(p) which describe this (in the Schrodinger equation) and both follow from A=-Et+px for classical and quantum free particle mechanics. Thus though one cannot measure x and p exactly simultaneously in quantum mechanics, the dynamics e.g. exp(ipx) contains exact values of both in the probability. We argue that statistical quantities seem to be linked to the microscopic dynamical variables.

Operator Entropies

In (2) operator entropies are mentioned i.e. one may write <B> = Tr (d B) where Bij = <i B j> and d is the probability a*i aj where W(x) = Sum over i a(i) W(i) and <B> = < W B W>. If B is diagonal in some set |i> then a*i ai is the probability for this state. If one considers a pure bound state, one may set |i>=exp(ipx) b where b is a normalization factor. Then. < W pp/2m W> = Integral dp pp/2m a*(p)a(p) ((4)). If one tries to create a Shannon's entropy linked to these eigenstates then:

Sp = -Integral dp a*(p)a(p) ln(a*(p)a(p))   (5))

((4)), however, is obtained by integrating out x in order to obtain a probability $P(p)=a^*(p)a(p)$. One may ask: Why does one integrate out one variable of the two dynamical pair p,x in order to obtain a preferential entropy ((5))?

For example, if one decides to focus on x. The $<W\ KE\ W>$ = Integral dx $W^*(x)W(x)$ $(-1/2m\ d/dx\ dW/dx)$ / W and $P(x) = W^*(x)W(x)$ yielding:

Sx = - Integral $W^*(x)W(x)\ \ln(W^*W)$ ((6))

The same operator (kinetic energy) is associated with two different entropies because one insists on integrating out one variable in order to find a probability based on the other.

Consider a hand-way scenario. Imagine that one has p values, p1, p2 and p3 with weights a(p1), a(p2) and a(p3). Any permutation of the a()'s leaves ((5)) unchanged, but W(x) changes for each permutation. Furthermore average kinetic energy changes as does overall energy. This begs the question: Why does the same Sp represent three very different systems?

 The first law of thermodynamics $dE=TdS - PdV$ involves E. En for a single bound state follows from the solution of the time-independent Schrodinger equation. This, however, is an equation in W = Sum over p $a(p)\exp(ipx)$ not in P(x) and P(p). It is the dynamics of W(x) i.e. the exp(ipx) a(p) which govern this system. Changing E through a quantum adiabatic change of box size L (single particle in a box with infinite potential walls) changes W(x), but in a scaled way. Keeping exp(ipx) fixed as $x\rightarrow x/L$ means $p\rightarrow pL$. From ((3)) it may be shown that Sp goes as ln(L) and Sx as ln(1/L) so a sum of Sp and Sx would make the quantum adiabatic change isentropic. This shows that a quantum adiabatic change involves both x and p. How is this linked to a probabilistic scheme?
    Instead of using P(x) or P(p) alone in Shannon's entropy, we argue as in (4) that one may use: P(x)P(p/x) where P(x)=WW and P(p/x)=a(p)exp(ipx)/W for a bound state. Then Shannon's entropy becomes:

S = Sp + Sx ((7))

 (This is the identical result to using P(x)P(p). If one uses P(x)P(p/x) there is a term ipx exp(ipx)a(p)W(x) which integrates to zero.)

W(x)=Sum over p a(p)exp(ipx) So Why Are Changes in a(p) Not Enough?

   Consider a particle in a box with infinite potential walls. En = b nn/LL where b is a constant and n the energy level. A quantum adiabatic change occurs so n remains constant so dEn changes as dL. The wavefunction changes as well, but TdS should not. Thus providing changes in a(p) immediately yields the new wavefunction W(x, L+dL), but TdS should represent a function of probabilities which does not depend on L. Thus an entropy based on a(p) alone is not sufficient.

Thermodynamics and Large N

For a particle in a box with infinite potential walls, $W(x) = 1/\sqrt{L}\, f(x/L)$ and $a(p) = \sqrt{L}\, f(p)$. Thus one may create Shannon's entropy form for probabilities WW and $a(p)a(p)$ using ln in order to obtain $\ln(1/L)$ and $\ln(L)$ so that these cancel. In other words no large N assumption is needed. It is noted in (2) that the standard view from classical statistical mechanics is that one has a large N system [so that ln (factorial counting schemes) using Stirling's approximation yields Shannon's form]. It is also noted that thermodynamics matches this large N approximation. Here we note that there are ways to obtain Shannon's form e.g. linearity, removal of L box from entropy etc which make no use of large N assumptions.

Conclusion

In conclusion we argue that one may link quantum dynamics to x and p already at the classical action $=-Et+px$ level (for both free relativistic and nonrelativistic particles). X and p are part of classical dynamics and classical statistical entropy and given that x and p are part of quantum dynamics of $W(x)=$ Sum over p $a(p)\exp(ipx)$ and that En follows from a solution of the Schrodinger equation using $W(x)$ we argue that both p and x should be part of a quantum bound state entropy. We further argue that one may use the probability $P(x)P(p/x)$ in Shannon's entropy form which yields the same integrated result as using $P(x)P(x)$ i.e. $S=Sp+Sx$. This ensures that for a pure bound state, a quantum adiabatic change in a parameter (i.e. work) leaves S constant. Thus we argue against the idea that one must only use operator specific entropies only. For a bound state we suggest focusing on the dynamical variables p and x and calculating a Shannon's entropy which includes both i.e. $S=Sp+Sx$.

References

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