The Schrodinger Equation and Maximum Entropy

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Given that quantum mechanics is argued to be a statistical theory, there have been attempts to investigate if the Schrodinger equation follows from the maximization of Shannon's entropy. For example in (1), Shannon's entropy using P(x)=density is maximized subject to energy constraints and the Schrodinger equation appears in the zero temperature limit. Furthermore, traditionally it is argued that the free particle quantum wavefunction exp(ipx) has a modulus of 1 at all x points, which seems to be a statement of maximum entropy. If that is the case, how does exp(ipx) follow from the maximization of entropy ? In this note, we try to examine the role of maximum entropy in the Schrodinger equation and specifically argue that two principles are used. First, maximization of entropy using conditional probability not P(x) is applied using an xW (W=wavefunction) and not energy constraint. Secondly, Newton's conservation of energy is applied to a quantum ensemble of free particle conditional probabilities obtained in the first step. Thus, statistical arguments are only part of the quantum picture.

The Schrodinger Equation as a T=0 limit of a Maximization of Entropy Equation (1)

In (1), the Schrodinger equation appears as the zero temperature (Lagrange multiplier) of a maximization of entropy given by:

density(x) ln[density(x)/density0(x)] + b1 density(x) + b2 H density(x)   ((1))

where density0(x) is a prior and H the energy. The result is:

density(x) = density(0)/Z exp(-H/T) where Z= Integral dx density0(x) exp(-H/T) ((2))

In (1), it is further shown that using density= W* W (W=wavefunction), ((2)) can be shown to be the solution of a Schrodinger type equation which becomes the actual Schrodinger equation if T=0. No new assumptions are needed, so this approach suggests that the Schrodinger equation follows from a maximization of a Shannon's entropy -P(x)ln(P(x)) using P(x)=density(x) in the T=0 limit. The fundamental point, however, is that this Schrodinger equation is expressed as:

HW = E W ((2b))

In particular, H is an operator representing energy, but no proof is given that average kinetic energy is of the form -1/2m d/dx d/dx W / W. ((2b)) as it stands is a classical equation. In this note, we argue that statistical maximization of entropy may be used to demonstrate that -1/2m d/dx d/dx W / W is the form of kinetic energy at x i.e. Sum over p pp/2m P(p/x), but that ((2b)) is a Newtonian and not statistical statement.

Classical Mechanics

It is possible to define a classical density (2):

$P(x) = Cdt = Cdx/v(x)$ ((3))

for a classical bound state, where $v(x)$ is the velocity i.e. $.5m\,v(x)v(x) + V(x) = E$. ((4))
which is a consequence of Newton's second law. If one forms a Shannon's entropy expression
i.e. $C/v(x)\ln(C/v(x))$ and maximizes by varying $v(x)$ subject to
Integral dx $C/v(x)$=constant1 and Integral dx $.5mv(x)v(x)C/v(x) + V(x)C/v(x) = E\,C$ then:

$1/v(x) = $ density$(x) = \exp[-b\,(\,mv(x)v(x)/2 + V(x))\,]$ where b is a Lagrange multiplier ((5))

Thus, density(x) is given by a Maxwell-Boltzmann type expression, but this is not the Newtonian
solution of the problem. Furthermore, b is given by solving for the constraints and so it does not
follow that one would take b=0. Thus, ((5)) matches the result of ((1)), but it seems that $v(x)$
follows from Newtonian mechanics and not statistics.

Correspondence Principle

According to the correspondence principle, in the high energy limit, quantum density
$W^*(x)W(x)$ (which has crests and troughs) has an envelope function which roughly matches
$1/v(x)$. If $v(x)$ follows from Newton's law (or the conservation of energy equation) and not from
the maximization of Shannon's entropy, one would expect the same for at least for the envelope
of quantum bound density $W(x)W(x)$ (as $W(x)$ is real). Thus, at least part of the quantum does
not seem to be based on maximization of entropy, but rather Newtonian mechanics.

Quantum Free Particle Probability

In the above two sections, we argue that Newton's second law and not maximum Shannon's
entropy [using $P(x)$] seems to govern the classical density $= C/v(x)$ and the envelope of the
quantum bound density $W(x)W(x)$. This idea should hold for a free quantum particle i.e. one for
which $V(x)=0$. In such a case, $W^*(x)W(x)$, the envelope should be a constant. This follows also
from the idea of maximization of entropy, however i.e.:

$P(x) =$ density$(x) = C\exp(-.5mvv)$ where $v(x) =$ constant ((5))

Thus, in the free particle case, both Newton's law and the maximization of Shannon's entropy
with $P(x)$ both yield a constant density. This is not surprising as a particle moving with a
constant speed has an equal probability to be at any x point and in classical statistical
mechanics, each x point has the same probability if there is no potential. The physical situation
in statistical mechanics is different, however, because there exists two-body scattering which
does not depend on x if there is no $V(x)$. This, however, is equivalent to a particle having the
same velocity at two different points. In other words, statistical mechanics is linked to Newtonian

mechanics as the MB distribution is C exp[- (.5mv(x)v(x) + V(x))/T] where E= .5mv(x)v(x) + V(x) follows directly from Newtonian mechanics and not the maximization of entropy. Conservation of energy in statistical mechanics is a property which exists outside of the statistics of the problem. (Furthermore, the MB distribution makes use of the idea of elastic scattering which again is related to conservation of kinetic energy and not statistics.) The statistical aspect enters through a balancing of forward and backward reactions.

   The "wavefunction" for a free quantum particle is exp(ipx). Traditionally it is argued that this wavefunction has a modulus of 1 at all x points which seems to indicate that more complicated issues exist. First, the statement that the modulus of exp(ipx) is 1 suggests that P(x)=constant at all x points. Thus, exp(ipx) is like " a kind of square root" of P(x) or at least linked to probability. We call it at relative conditional probability and move away from the idea of using P(x) in forming Shannon's entropy.

   Secondly, we suggest there is possibly a "principle" in quantum mechanics linking conditional probability changes for a free particle (or even a bound one) and average momentum (3). For a free particle, the momentum is the constant p. If this principle is to hold, one should expect it to be present as a constraint in any maximization of entropy expression. We try to show that this "principle" seems to follow from using a constraint of xW and maximizing Shannon's entropy using conditional probability W(x) :

-W ln(W) - b xW →   -ln(W) -1 -b x = 0   ((6))

Then W(x)=Cexp(-bx). The solution should not grow or decrease and its derivative should be proportional to p, momentum so:

 W(x)= Cexp(ipx)   ((7))

It is interesting to note that integral pdx (0, 2pi) px cos(px) = 0, but iIntegral dx (0, 2pi) x sin(px) = i. Thus, Real Integral x W dx = 0 over the cycle x=0 to x=2pi. Thus, there seems to be some fluctuation within (0,2pi), but overall the average real part of Integral x W(x) dx is 0. This seems to be linked to uncertainty in x as the average is 0, yet there are probabilities to have x at different places in the interval, some with positive and others with negative conditional probabilities. It should also be noted that the size of the interval depends on p i.e. p=2pi/L, L being the wavelength or interval size.

If one tried to establish a similar equation using W*W instead of W, then integral dx xW*W is automatically 0 by symmetry. Alternatively, one may use P(x) in Shannon's entropy subject to the constraint Integral P(x) dx =1. This yields P(x) = constant. Given that one wants x dependence, one may argue that a solution is P(x)=W*(x)W(x) with W(x) = exp(iG(x)) and then go on to argue that G(x)=px is a solution with a flow proportional to p. It seems, however, that one should be able to maximize entropy related to W directly as an alternative.

As a result, we argue that the maximization of entropy used in quantum mechanics is quite different from the usual maximization of Shannon's entropy of the real P(x)=density(x) subject to energy constraints.

It is immediately seen that: d/dx exp(ipx) = ip exp(ipx) and that -d/dx d/dx exp(ipx) = pp exp(ipx).   ((8))

Thus, the conditional probability is directly linked to probability values for p (momentum) and pp (related to kinetic energy).

Quantum Bound State with V(x)

   In the above section, we argue that maximization of Shannon's entropy using the conditional probability W(x) yields the free particle wavefunction exp(ipx) if one uses xW as a constraint which leads to a flow result: -id/dx W = p W. That next consideration is the presence of a potential V(x).
   Let us assume one wishes to use exp(ipx) (the free particle wavefunction) in a problem with V(x). In such a case, V(x)= Sum over k V(k) exp(ikx) is the stochastic collision source instead of two body collisions in a classical gas. The rule for two body collisions in a classical gas is the existence of a reaction time reversal balance i.e.

P1+p2 → p3+p4 and p1p1/2m + p2p2/2m = p3p3/2m + p4p4/2m ((9))

with   f(p1)f(p2)=f(p3)f(p4)   ((10))

For a quantum bound state, the rule is completely different, namely:

KE ave (at x) + V(x) = E   ((10))

((10)) is a Newtonian statement applied to an average and does not necessarily follow from statistics. Thus, one needs a statistical expression for KEave(at x). This is where the maximum entropy exp(ipx) conditional probability expression comes into play because:

KE ave (at x) = [Sum over p pp/2m a(p) exp(ipx)] / W(x) where W(x)=Sum over p a(p)exp(ipx)

Or KE ave (at x) = -1/2m d/dx d/dx W / w

   ((11))

Thus, the unknowns a(p) may be solved from ((10)) without any maximization of entropy. Maximization of entropy has already been performed to obtain exp(ipx) which yields a form for kinetic energy a(p) pp/2m exp(ipx). If a function differing from exp(ipx) had resulted, then -1/2m d/dx d/dx W / W would not be the average kinetic energy.

It is interesting to note that the average conservation of energy equation becomes a differential equation because of the form exp(ipx) i.e.

-1/2m d/dx d/dx W / W + V(x) = E   ((12))

This is a mathematical eigenvalue equation. For the case of distinct eigenvalues (and given boundary conditions), there is a unique set a(p) corresponding to an E. Thus, there does not seem to be a question of maximizing entropy to find an appropriate set of a(p)'s.

Reverse Argument

   Given ((12)), the Schrodinger equation and its limit V(x)=0, the solution exp(ipx)=W(x) follows from a maximization of entropy which does not use an energy constraint unlike the approach of (1) and traditional approaches. It seems energy conservation (applied to averages) differs from statistical maximization of entropy approaches. The contribution of the statistical approach is to give the form of the average kinetic energy at each x point. Then, a separate approach, i.e. Newton's conservation may be applied to determine any unspecified constants. In general, one would combine these two i.e. if conservation of average energy is a constraint it may be incorporated in the entropy expression to be maximized, but this cannot be done if one does not know the form of average kinetic energy at x in terms of W(x) the conditional probability.

Conclusion

   In conclusion, we argue that maximization of Shannon's entropy using a conditional probability for a free particle may be performed if one uses xW as a constraint which leads to exp(px) without using an energy constraint. This result is equivalent to -id/dx W = p W, so the flow condition seems to follow from maximization of entropy. This is peculiar and differs from standard approaches which use density = W*W = P(x) in Shannon's entropy and obtain HW=EW type equations in certain limits without proving that -1/2m d/dx d/dx W / W is average kinetic energy, we argue. The approach of using W in Shannon's entropy and the constraint xW seems to lead to a kind of fluctuating picture with x uncertainty. On average x is 0 i.e. Real Integral dx x exp(ipx) is 0 for (0, 2pi), but x has values with positive and negative conditional probabilities. This is similar to the idea that exp(-ipx)exp(ipx) = 1 at all x, yet there is periodic motion beneath the constant density "surface".
   A key point to obtaining exp(ipx) as a conditional probability is that it allows for the formation of kinetic energy at x i.e. Sum over p pp/2m P(p/x) in a relatively simple manner from W(x) where P(p/x)= a(p) exp(ipx)/W(x). In other words, W(x) represents an ensemble of free quantum particles. One may apply the rule that average energy at x is E, but still requires an explicit expression for average kinetic energy at x. If one knows the conditional probability function at x which depends explicitly on exp(ipx), this may be done. exp(ipx), in turn, may be obtained from a somewhat peculiar maximization of entropy dependent on a flow constraint d/dx W = ip W.

Thus, the Schrodinger equation is, we argue, a combination of maximum entropy applied to obtain exp(ipx) and Newton's conservation of energy applied to ensemble averages.

References

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