

Alternative Expression for Entropy in Quantum Mechanics?

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Recently, there has been some interest in the literature in calculating temperature dependent quantum mechanical wavefunctions using the principle of maximum entropy. The idea seems to be to obtain a differential equation, similar to the Schrodinger equation, but with temperature dependent terms. It should be noted that this does not follow von Neumann statistical quantum mechanics. It should also be noted that other authors in the literature maximize or minimize other quantities related to information theory to calculate a wavefunction. The objective of this note is not to examine the maximization of entropy as applied to the calculation of a wavefunction, but to suggest a different form for entropy. Traditionally, authors seem to use the Shannon form $-k W^*(x)W(x) \ln[W^*(x)W(x)]$ as a spatial entropy and exchange $W(x)$ for $f(p)$ for the momentum one, with $W(x)$ being the wavefunction. It is the spatial form which they seem to maximize in calculations. In this note, we consider a probability $P(x \text{ intersection } x) = W(x) f(p \sin(px))$ and use it in Shannon's entropy. Maximization of entropy then leads to an integral equation which, it seems, needs to be solved numerically. We can however, multiply such an equation by $f(p)$ and sum over p to obtain results which can be compared with those of authors who use $-k W^*(x)W(x) \ln[W^*(x)W(x)]$.

Some Current Maximum Entropy Calculations in the Literature

In (1), the authors maximize:

$$-W^*W \ln[W^*W/d] + b_1 W^*W + b_2 W^* H W \quad ((1))$$

Here $W(x)$ is the wavefunction, $d(x)$ a prior which needs to be set, although it ends up being 1 for some calculations, H the Hamiltonian and b_1 and b_2 Lagrange multipliers. In (1), ((1)) is maximized subject to W^* and W and the following result proposed:

$$HW + T W \ln[W^*W/d(x)] = q W \quad ((2))$$

where q is a constant and T , the temperature another constant arising from a Lagrange multiplier.

The authors of (1) then consider various Hamiltonians H and often obtain numerical solutions to ((2)). In particular, for a particle in a box with $H = -1/2m \text{ del}^2$, the authors obtain a numerical result. It is suggested in this note, that for a particle in a box, the ground state solution of an oscillator $W(x) = \exp(-ax^2)$ satisfies ((2)) as $d(x) = 1$ and $\ln(W^*W) = -ax^2$ the oscillator potential.

In (2), we tried to argue that one might be able to use an equation like ((2)) to describe a particle in a box subject to a temperature. We did not maximize entropy but suggested that f_p , the momentum wavefunction, should be $\exp(-p^2/2mT)$ if equilibrium occurred.

Probability Considerations

It seems that $P(x)=W^*(x)W(x)$ and $P(p)=f_p^*f_p$ in the literature where f_p is the Fourier transform of $W(x)$ in quantum mechanics. In (3) we noted that the time-independent Schrodinger equation could be written as:

$$[\text{Sum over } p \ p^2/2m \ f_p \sin(px)] / W(x) + V(x) = E \quad ((3))$$

and define: $P(p/x)=f_p \sin(px) / W(x)$. Given that $P(p/x)=P(x \text{ intersection } p) / P(x)$, we suggest that one can consider:

$$P(p \text{ intersection } x) = W(x) f_p \sin(px) \quad ((4))$$

We suggest that this represents a quasiparticle plane wave type solution that exists in a quantum bound state. These various quasiparticles are being stirred up by the potential, i.e. the potential scatters the particle into these states. f_p is related to having a momentum of p , $\sin(px)$ models zitterbewegung (forward- backward motion) and $W(x)$ is a position changing amplitude. It should be pointed out that $P(p \text{ intersection } x)$ can be negative, but this will only affect one term in our results, related to $\ln(\sin(px))$. In information theory, $\ln(\text{Probability})$ is related to information. $\sin(px)$ can be positive or negative, we argue in (4), depending on how the zitterbewegung particle interacts with the potential. If the "information" for forward and backward zitterbewegung are the same, as implied by the symmetry of $\sin(px)$, it might be possible to use $\ln[|\sin(px)|]$ when calculating Shannon's entropy using ((4)).

Thus we suggest using a Shannon's entropy of the form:

$$-W(x) f_p \sin(px) \ln\{ W(x) f_p \sin(px) \} \quad ((5))$$

Maximization of Entropy

The form ((5)) can be maximized (actually we find a stationary point) by using Lagrange multipliers b_1 for $\langle W|H|W \rangle = E$ and b_2 for $\langle W|W \rangle = 1$ and writing ((5)) solely in terms of f_p with:

$$W(x) = \text{Sum on } p \ f_p \sin(px).$$

This seems to lead, by varying f_p , to:

$$B^2 2f_p + b_1 f_p [p^2/2m + V(x)] + \int dx \sin(px) W(x) \ln\{\sin(px)\} \quad ((6)) \\ + f_p \ln(f_p) + \int dx W \ln(W) \sin(px) + 2f_p = 0$$

This is a somewhat complicated equation compared with ((2)) and appears to be an integral equation as $W(x) = \int dp f_p \sin(px)$ for one dimension. As a result, one would need to find numerical solutions, which is not done in this note.

One may ask, however, if one can compare the result of ((6)) with that of ((2)), obtained using $W(x)W(x) = P(x)$ in Shannon's entropy.

If one multiplies ((2)) by $W(x)$ and integrates (assuming $W(x)$ is real for this scenario) one obtains:

$$\langle W|H|W \rangle - T \{ \int dx \text{ Shannon's space entropy density} \} = q \langle W|W \rangle$$

Let us call $\{ \int dx \text{ Shannon's space entropy density} \} = S_x$ or spatial entropy as it seems to be called in the literature.

On the other hand, multiplying ((6)) by f_p and summing of p seems to yield:

$$B^2 + b_1^2 \langle W|H|W \rangle + .5 S_p + .5 S_x + \int dx \{ W(x) \sum_p f_p \sin(px) \ln(\sin(px)) \} \quad ((7))$$

One can perhaps use $|\sin(px)|$ in the argument of \ln .

Here S_x is the spatial Shannon's entropy and S_p the momentum one, namely:

$$2 f_p \ln(f_p).$$

The integral in ((7)), may perhaps be described as an entropy related to zitterbewegung. Thus, ((7)) contains three kinds of entropy, spatial, momentum and zitterbewegung and is not or a completely random form, but seems to parallel equation ((2)), but deal with three different entropies present in the system. In quantum mechanics, momentum and position are related and interference occurs, perhaps due to zitterbewegung, so it is interesting to see all three present.

Conclusion

In conclusion, we suggest using $P(x \text{ intersection } p) = W(x) f_p \sin(px)$ in the calculation of Shannon's entropy for problems which maximize entropy in quantum mechanics. Normally in the literature, people use $P(x)$ in Shannon's entropy. We obtain a somewhat complicated integral equation which can be computed numerically instead of simpler Schrodinger type equation obtained by using $P(x)$. (Solutions of the Schrodinger type equation however have to

be often numerically computed.) By multiplying the integral equation obtained in this note by ψ and summing over ψ , we obtain:

$$B^2 + b_1^2 \langle W|H|W \rangle + .5 S_p + .5 S_x + \int dx \{ W(x) \sum_p \psi(p) \sin(px) \ln(\sin(px)) \}$$

Which is very similar to the result using $P(x)$ in Shannon's entropy, but with three entropy terms: S_x spatial entropy, S_p momentum entropy and $\int dx \{ W(x) \sum_p \psi(p) \sin(px) \ln(\sin(px)) \}$ a kind of zitterbewegung entropy instead of just S_x obtained from a $P(x)$ in Shannon's entropy calculation.

References

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