

Complex Probabilities with Phase in Bound State Quantum Mechanics

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Bound state quantum mechanics is formulated as a statistical theory in which averages seem to be given by the recipe: $\langle B \rangle = \int dx W(x) B W(x)$ where $W(x)$ is the wavefunction and B an operator. If B is strictly a function of x , the $\langle B \rangle = \int dx d(x) B(x)$, where $d(x) = W(x)W(x)$ is the spatial density and the recipe is exactly of the form of statistical mechanics. In the case that momentum is present, it is represented by $i\hbar d/dx$ operating on $W(x)$ and so matters differ from classical statistical mechanics. In this note, we try to express bound state quantum mechanics in terms of complex probabilities (with phase) and show how absolute $P(x)$, $P(p)$ probabilities and also conditional $P(x/p)$ and $P(p/x)$ appear in the theory. We then suggest that it is $P(x \text{ and } p)$ that is important and show this has implications on entropy. In an earlier note, we described an entropy in such terms, but instead of using $\exp(ipx)$ as part of the probability, $\sin(px)$ was used to keep probabilities real. In this note, we suggest probabilities should be kept complex and shows this leads to a real expression for entropy. For the case of the ground state oscillator, this expression collapses to a sum of momentum entropy $2\pi \ln(\pi p)$ and spatial entropy $2W(x) \ln(W(x))$, where π is the Fourier transform of $W(x)$.

Traditional Description of Bound State Quantum Mechanics

Traditionally, quantum mechanics is described as a statistical theory, but it is formulated in a manner which makes it difficult to compare with classical statistical mechanics and classical mechanics. Note: Classical mechanics may be formulated with $d(x) = 1/v(x)$ where $d(x)$ is density and $v(x)$ velocity at given by conservation of energy $.5mv(x)v(x) + V(x) = E$. Quantum mechanics, however, matches classical statistical mechanics for the ground state oscillator and classical mechanics for high energy eigenvalues for all potentials. Thus, it seems there should be clear link between quantum mechanics and other statistical theories.

Bound state quantum mechanics assumes a function $W(x)$, called the wavefunction. $W(x)W(x)$ is stated to be equal to the spatial density and measurements appear to confirm this accurately. The Fourier transform of $W(x)$, π , when multiplied by itself $\pi^* \pi$ yields the probability for a particular momentum p . It has often been asked why $W(x)$, the square root of probability, is used in a statistical theory.

To calculate expectation values, one considers operators which are combinations of x functions and $(d/dx)^n$. Given an operator B , the average value is given by:

$$\langle W(x) | B | W(x) \rangle \text{ where } W(x) \text{ is real for bound states. } ((1))$$

It should be noted that for $B(x)$ as a function of x alone, $((1))$ is identical to the classical statistical mechanical result $\int dx d(x) B(x)$ where $d(x)$ is density. Thus, quantum effects

seem to appear when B contains d/dx derivatives and operates directly on the “square root of probability” i.e. $W(x)$.

Bound State Quantum Mechanics with No Potential

To attempt to see what is occurring, first consider the case of a particle in a box with no potential. In such a case, the particle has kinetic energy $p^2/2m$ and can be moving forward or backward, i.e. momentum is p or $-p$. In classical mechanics there would be a constant density, but not in quantum mechanics. We suggest this is due to the idea that a quantum particle is not a point, but is cycling $E = \hbar^2 k^2 / 2m$, and is represented by $\exp(ikx)$. $\exp(ikx)$ is complex and seems to suggest that even for one dimension, there is a second dimension in the problem. For a particle moving in one direction, this cycling is present, but does not really affect average momentum $\exp(-ikx) \hbar(ik) \exp(ikx)$, kinetic energy or even density $\exp(ikx)\exp(-ikx)$. If one places such a particle in a box with an infinite potential at each wall, but otherwise no potential, the particle can bounce back and forth. In order to determine density or average values, it seems one must wait quite some time. In other words, we argue that bound state quantum mechanical averages are taken over a cycle time of the order of $1/E$. For the oscillator ground state, this can be of the order of the mechanical period, which is a large time compared to measurement time in classical mechanics.

Traditionally, in bound state quantum mechanics one adds the wavefunction $\exp(ikx)$ for the particle moving in the forward direction to $\exp(-ikx)$ for backward motion. The complex portions cancel. One might think of this as a kind of average. A $2\cos(kx)$ term is left. Then, one uses the recipe of squaring this sum to find the spatial density.

Here, we try to think in terms of probabilities and conditional probabilities. We know that there are two momenta p and $-p$ and we expect them to have equal weights due to symmetry. Let us ask what the probability is to find a p given that one is at x . We suggest:

$$P(p/x) = C f_p \exp(ipx) / \cos(px) \quad ((2))$$

Here f_p is a momentum weight, C is some constant, the box extends from $-L/2$ to $L/2$ and $\cos(px)$ is simply a normalization constant. We note that f_p is the Fourier transform of $\cos(px)$. Thus, we suggest that the cycling feature of a quantum particle is actually important in averages. At different x points, there are different real and complex portions $\cos(kx)$ and $\sin(kx)$. The $\sin(kx)$ cancel for p and $-p$, but the $\cos(kx)$ do not and $\cos(kx)$ has different values at different x . If one sums $P(p/x)$ for all p one obtains 1 as expected as $f_p = f_{-p}$. If one wants to calculate an average value of momentum function at x , then one can write:

$$p^n P(p/x) \quad ((3))$$

$$\text{If } f_p = f_{-p}, \text{ then } ((3)) \text{ is equivalent to } C f_p / \cos(px) (d/dx)^n [\exp(ipx) + \exp(-ipx)] \quad ((4))$$

Next, consider the slightly more complicated $P(x/p)$. This suggests that if one has a momentum p , it will have different probability values to be at one x point versus another. This seems to be related to the fact one is taking a long term average and having imaginary $\sin(kx)$ terms “cancel”. In addition, at a point x one has a phase $\exp(ipx)$. Thus, a form which mimics ((2)) is:

$$P(x/p) = C \cos(px)/f_p \exp(ipx) \quad ((5))$$

Here, f_p is a normalization constant and $\exp(ipx)$ shows there is a difference in probability for p and $-p$. $\cos(px)$ gives spatial dependence, but is the same for p and $-p$. This $\exp(ipx)$ phase, which makes the probability complex, is important as:

$$\text{Sum over } p \ P(x/p) = C \cos(px)/f_p \ 2\cos(px) \quad ((6))$$

Thus, one obtains a $\cos(px)\cos(px)$ result, instead of a $\cos(px)$ which one might have expected had the phases not come into play. It comes into the long term average because the phase of each momentum is important in calculating the average as different momenta have different real and imaginary values at x .

Let us next consider the idea of spatial density. In a classical statistical gas with many particles, it is simply the number of particles in a volume which is considered to be constant over time. For a classical mechanical particle moving according to $.5mv(x)v(x) + V(x) = E$, it is the “number of particles” in a Δx in a fixed amount of time Δt . A slow particle may spend the entire Δt moving through Δx and so would have a count of 1. A fast particle would move through in a fraction of Δt and so for part of Δt there would be 0 particles in Δx , causing the so-called density to drop.

What is happening for the quantum particle moving back and forth? We try to define the density as:

$$d(x) = \text{Sum over } p \ P(x/p)P(p) \quad ((7))$$

Now, $P(p)$ does not depend on x and is the same for p and $-p$ we assume. Then, from the ideas above: $d(x)$ is proportional to $\cos(px)\cos(px)$ which is the $d(x)=W(x)W(x)$ result of quantum mechanics.

P(x and p) Probability

In the above discussion, $d(x)$ was obtained by summing $P(x/p)P(p)$ but this is equivalent to:

$$P(x \text{ and } p) = W(x) f_p \exp(ipx) \quad ((8))$$

We suggest, as in (1), that ((8)) may be the important probability to consider when performing Shannon entropy calculations. In (1), in order to avoid complex probabilities, $\exp(ipx)$ in ((8))

was replaced with $\sin(px)$ (or $\cos(px)$ depending on symmetry). This is an error, we think, and suggest using ((8)). Consider now Shannon's entropy:

Shannon's entropy = Sum over i $P_i \ln(P_i)$ where $P_i = P(x \text{ and } p)$

= Sum on x and p $W(x) f_p \exp(ipx) \ln [W f_p \exp(ipx)]$

= Sum on x $W(x)W(x) \ln(W(x))$ + Sum on p $f_p f_p \ln(f_p)$ + i Sum on x and p $W(ipx) f_p \exp(ipx)$ ((9))

The first two terms in ((9)) are related to spatial and momentum Shannon's entropies. The third term looks complex, but if $f_p = f \cdot p$ becomes $W(x) \times d/dx W(x)$, thus:

Shanon's entropy = C_1 Sum on x $W(x)W(x) \ln(W(x))$ + C_2 Sum on p $f_p f_p \ln(f_p)$ + C Sum on x $W(x) \times d/dx W(x)$ ((10))

Here we use the idea that $W(x) = \text{Sum on } p f_p \cos(px)$. C, C_1 and C_2 are constants.

For the ground state of a harmonic oscillator Sum on x $W(x) \times d/dx W(x)$ for $W(x) = \exp(-ax^2)$ yields, $\exp(-2ax^2) 2ax^2$. This is proportional to Shannon's entropy for space i.e. $2W(x)W(x)\ln(W(x))$. It was shown in (2), that energy for the ground state oscillator could be written as a linear combination of momentum entropy and spatial entropy because the third term in ((10)) is proportional to spatial entropy.

Momentum and Spatial Probabilities

Bound state quantum mechanics seems to rest on averages of momentum terms and spatial terms. Consider classical kinetic energy $.5 m v(x)v(x)$ with $.5mv(x)v(x) + V(x) = E$. In quantum mechanics, $.5 m v(x)v(x)$ is obtained as a long term average at each point x . Since this involves a momentum average, the conditional probability $P(p/x)$ is used and the wavefunction comes into play i.e.:

$[\text{Sum over } p \quad p^2/2m f_p \cos(px)] / W(x) = .5 m v(x)v(x)$ ((11))

Thus, a classical deterministic result $.5 m v(x) v(x)$ is obtained through a long term average in quantum mechanics. Note that ((11)) uses f_p and not $f_p \cdot f_p = P(p)$. Here conditional probabilities are needed.

If one decides to take a "second" average over space, it is defined in the classical statistical mechanics manner, namely:

$$\int dx \psi^*(x) \psi(x) \frac{1}{2m} \nabla^2 \psi(x) = \int dx \psi^*(x) \psi(x) \sum_p \frac{p^2}{2m} f_p \cos(px)$$

$$= (-1/2m) \int dx \psi^*(x) \nabla^2 \psi(x) \quad ((12))$$

Thus, one may see how certain quantum mechanical averages are really double averages, one first with momentum and a conditional probability, followed by a usual spatial density average. Incidentally, ((12)) is equivalent to:

$$\sum_p \frac{p^2}{2m} f_p \quad \text{where } f_p = P(p), \text{ the momentum probability. } ((13))$$

Thus, f_p alone appears in conditional probability averages, while $P(p)$ can appear in global average.

((13)) looks like the result for a classical statistical mechanical gas, but one does not maximize entropy here as ((13)) must match $\int dx \psi^*(x) \psi(x) \frac{1}{2m} \nabla^2 \psi(x)$ where $\psi(x)$ is completely dependent on the potential $V(x)$ and $\psi(x)$ is the Fourier transform of f_p .

Conclusion

In conclusion, we have considered bound state quantum mechanics in terms of complex probabilities and have tried to gain some insight into why density is $\psi^*(x)\psi(x)$. In some previous notes, we considered similar ideas, but strictly with real probabilities, which seems to lose the idea of the effect of complex phases on probability. In addition, we have tried to show how Shannon's entropy using the complex $P(p \text{ and } x)$ seems to lead to a linear combination of Shannon's entropy for momentum, Shannon's entropy for space and a term $\psi^*(x) \nabla^2 \psi(x)$.

References

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