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Density Operators and Time

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Abstract Our understanding of time from physics is through the combination of quantum mechanics and relativity. In quantum mechanics, measurements are represented by operators. The state of a system is usually represented by a wave function which is operated on by the operators. This view of time is compatible with relativity in that each event is assigned a unique time coordinate; the wave function changes with time. The only difficulty is the measurement or collapse process; this process must act outside of time as, in the language of special relativity, it modifies our representation of a single event, for example, a particle experiment, converting our representation from a wave to a particle.

The density matrix and density operator formulation of quantum mechanics is an alternative formulation that is compatible with all the old results of wave functions. It has certain advantages over the usual formulation and it gives a different view of time, one that suggests that our usual understanding of time in physics is over simplified.

We show that density formalism suggests an additional parameter in quantum states giving the time of the observer. And we show that the non Hermitian extension of density matrices give quantum states which include an arrow of time.

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1 Complex Phases

Let $\psi(x, t)$ represent a particle state. For this section, this will be a complex function of space x , and time t . The picture of the particle implied by the

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wave function picture is that of a wave which changes with time. At the time $t = t_0$, it is natural to think of the particle as being represented by the complex wave $\phi(x) = \psi(x, t_0)$. As such, the quantum wave function picture of a particle wave is analogous to the classical description of a wave function; the wave function of a single particle has a structure no more complicated than a movie, it consists of a series of still frames, each of them independent.

A wave function can always be multiplied by an arbitrary complex phase without changing the state represented. Rather than using $\psi(x, t_0)$ to represent the particle at time t , we may as well use $-\psi(x, t)$, $i\psi(x, t)$, etc.; any observable is unchanged when the wave function is multiplied by a complex phase. The situation is similar when one considers multiparticle states; the state vector formalism of quantum mechanics appears to supply a single-valued description of a particle state at a given time but the arbitrary complex phase is always there.¹

To convert a quantum wave function to a density operator, we take the product of the wave function with its complex conjugate:

$$\rho(x', t'; x, t) = \psi(x', t')\psi(x, t)^*. \quad (1)$$

Multiplying by the complex conjugate eliminates the arbitrary complex phase. Unlike the wave function, the density matrix is a uniquely defined mathematical object that we can associate with a quantum state. However, time appears twice in this object; the quantum state can no longer be thought of as a sequence of still frames in a movie. Instead, the wave function requires two space-time coordinates. And while the arbitrary complex phase is eliminated, the density operator is still complex; the complexity gives the difference in phase between two points in space-time. Instead of viewing a quantum state as a movie, a quantum state is a process. In fact, we can obtain a wave function representation of the quantum state from the density operator by choosing any arbitrary spacetime point (x_0, t_0) where the density operator is not identically zero, and setting:

$$\psi(x, t) = \rho(x, t)\psi(x_0, t_0), \quad (2)$$

and adjusting normalization appropriately.

2 Collapse

It's tempting to think of quantum collapse as a classical process similar to how we would describe the position of a particle moving in response to non deterministic or stochastic influences. After looking at the various things that could happen, assigning probabilities to them, we could end up with a probability density $p(x, t)$. As with the wave function formulation of quantum

¹ Wave functions, as representations of reality, can be replaced by their equivalence class under multiplication by arbitrary complex phases. This gives a unique representative of a quantum state, but it creates other problems such as the loss of linearity — the ability to add two states together to get a new state. And it gives no better understanding of the nature of time.

mechanics, we would be describing reality as a sequence of still frames, a movie.

The classical probability density $p(x, t)$ can be obtained from the quantum wave function ψ , or density matrix ρ as follows:

$$p(x, t) = \psi^*(x, t)\psi(x, t) = \rho(x, t; x, t). \quad (3)$$

From the point of view of the classical non deterministic particle description, the wave function is a sort of a square root. And from the density operator point of view, the classical probability density consists of the diagonal elements of the density operator.

A wave function must follow the Heisenburg uncertainty principle (HUP), which restricts how tightly one can spatially restrict a wave function with limited momentum. This restriction is built into the mathematics; one cannot construct a wave function $\psi(x, t)$ that violates the HUP even at a single moment in time. A physical explanation for the HUP is that the act of measuring the particle deflects it. For example, if we wish to use a bubble chamber to track the position of a charged particle, the collisions with the gas will deflect the particle and this will change its course. This is true before the experiment, but afterwards, we can determine the path the particle took by examining the track in the bubble chamber. The track has every appearance of a classical description of the particle.

For the case of the bubble chamber, collapse converts the quantum particle into a classical path. We can model this as a sharpening of the probability density $p(x, t)$. One can imagine $p(x, t)$ being so sharpened that it defines just a single path, but in any real experiment, even with a very good bubble chamber, we will have a more or less vague estimate of where the particle went and we will have to make do with a probability density.

This suggests that to understand collapse, we need a way of transforming the quantum description of the particle into a classical probability density, and then we need to sharpen that probability density in the same way that a classical probability for a non deterministic particle sharpens as the random events effecting the particle take place.

The collapse problem relates to the fact that the best description of a quantum event depends on the observer. But the dependence can be thought of in a simple way; if the observer's time T is less than the time of the event t , then the observer is looking at an experiment to be run in the future. In this case, the best description of the event is to use the wave function or density operator. And if $T > t$, then the best description is just the classical density $p(x, t)$.

To get this idea to work, we have to add T to the parameters for the density operator. Suppose that an observer at time $T = t - \tau$ represents the event as a wave function, and an observer at the later time $T = t + \tau$ represents the event as a classical probability. Then we can model the collapse of the wave function by adding the new variable T to the density matrix as follows:

$$\rho(x', t'; x, t; T) = \begin{cases} \rho(x', t'; x, t) & \text{if } t < T - \tau, \\ f(x', t'; x, t; T) & \text{if } T - \tau < t < T + \tau, \\ \rho(x, t; x, t) & \text{if } t > T + \tau. \end{cases} \quad (4)$$

where the middle function $f(x', t'; x, t; T)$ smoothly transitions from $\rho(x', t'; x, t)$ to $\rho(x, t; x, t) = p(x, t)$ in the interval $T - \tau < t < T + \tau$. The above is not a prescription for making predictions; the eventual probability density $p(x, t)$ is sharper than the HUP would provide so this is not possible. Instead, it's a description of how to get from the quantum description of the system, which requires phase information, to a collapsed description – without changing the nature of the mathematics.

3 A Reinterpretation of Bohmian Mechanics

We can slightly modify the ontology of Bohmian mechanics[3] using these principles. Bohmian mechanics was originally presented as a wave function theory but recently, the attraction of the density matrix approach has been appreciated in the literature.[1,2] Bohmian mechanics does not use an extra (observer) time variable T . Instead, a single particle quantum state is modeled with both a wave function and a classical particle path. The wave function follows the usual rules of quantum mechanics. The classical particle follows the probability current of the wave equation. The probability currents define flow lines that do not intersect, and that preserve probability density so we can suppose that if the particle was chosen from an initial density that matches the usual probability density of quantum mechanics, then the density will continue to obey the rules of quantum mechanics.

One of the intriguing variations of Bohmian mechanics assumes that there is some non determinism in the particle's path. This allows the probability currents to mix and so even if the initial probability density does not match the assumptions of quantum mechanics, as time goes on, the mixture will fill all states with their appropriate density. Another alternative is to suppose that the mixing is deterministic but chaotic. This variation of Bohmian mechanics provides the mathematical tools necessary to convert the density matrix to collapsed form.

Let's take the case where the particle begins at a single point in the probability density, say it is at x_0 at time t_0 . At some later time $t_0 + \tau$, the probability density widens out to the full quantum mechanical probability density $\rho(x, t_0 + \tau; x, t_0 + \tau)$. If the boundary conditions do not depend on time, say the particle is in a box, or we are modeling all the relevant particles as quantum states, then we can rewrite this process as that of a quantum state at fixed time t_0 , but looked at by observers with changing time T . When $T < t_0 - \tau$, the observer uses the full quantum mechanical description of the situation. As T increases to t_0 , the wave function collapses and the observer is left with a classical probability density. Finally, the particle ends up at x_0 .

David Bohm's ontology for Bohmian mechanics requires a preferred reference frame; otherwise the paths taken by the quantum particles depend on the choice of reference frame. Adding the variable T has a similar effect. To obtain Lorentz invariance, we have to assume that the laws of physics, other than wave function collapse, do not depend on T .

4 The Arrow of Time

Any spinor state can be converted into a density matrix but the reverse is not true. Since density matrices are more general, it's possible that a theory that is very complicated when written in the spinor language becomes simple when written in density matrix form.

The usual extension that density matrices provide over spinors are statistical mixtures. Less well known are the non Hermitian density matrices. These define states with an inherent arrow of time.

A way of defining the pure density matrices is that one takes all possible spinors, and converts them to density matrix form. This will provide the Hermitian density matrices only. These density matrices are characterized by three properties. First, they are idempotent, that is, they are projection operators and satisfy $\rho\rho = \rho$. Second, they have trace = 1. And finally, they are Hermitian. In defining the non Hermitian density matrices, we keep the first two characterizations, but remove the third.

Let ρ_u be the density matrix in the Pauli algebra for spin in the u direction. We will use:

$$\begin{aligned}\rho_{+z} &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \\ \rho_{+x} &= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.\end{aligned}\tag{5}$$

Then twice the product:

$$2\rho_{+z}\rho_{+x} = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix},\tag{6}$$

is a projection operator, and has trace = 1, but it is not Hermitian. More generally, the product of any two pure density matrices is a real multiple, possibly zero, of a not necessarily Hermitian density matrix. And in general, any density matrix, Hermitian or not, can be written as the real multiple of the product of two Hermitian density matrices in exactly one way.

The essence of the density matrix view of quantum mechanics is that quantum states are processes. Complex phases of quantum states are defined by the difference between the phase at one point in space-time and the phase at another. Non Hermitian density matrices generalize this principle from being a statement about the $U(1)$ symmetry of the complex phase, to being a statement about, in the above example, the $SU(2)$ symmetry of Pauli spin.

Instead of a quantum state having a specific complex phase or a specific spin at a specific time t , the (non Hermitian) density matrix approach defines the quantum state as being a process which defines the change in complex phase between two points, and the change in spin orientation between two points. As such, non Hermitian density matrices are the natural extension of density operators which correspond to the extension of the Abelian symmetry $U(1)$ to higher symmetries.

When one defines a non Hermitian density matrix as a product of two Hermitian density matrices such as $k\rho_u\rho_v$, for k some real constant, one is defining a quantum state which has an orientation in time. In the language

of spinors, such a state takes a quantum state v as its input and produces a quantum state u as its output. This can be a method of defining elementary particles which violate time symmetry.

5 Conclusion

The lesson from density formalism is that time is more complicated than it appears. In addition to the (x, t) of the usual space-time, there may be an additional time variable. We've written the above argument as if that time T is the time of the observer. However, in this model observers do not interact per se, and consequently we may as well make the simplifying assumption that all observers have the same T . Then T becomes an attribute of the universe as a whole, and an explanation for that persistent human insistence on free will and the uniqueness of the present.

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