Contextuality in a Deterministic Quantum Theory

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I would like to dedicate this thesis to my mother, who introduced me to the most valuable notion, that of freedom, and to my father who fostered it.

Declaration

The work presented in this dissertation has been carried out by me under the guidance of Prof. Arvind, at the Indian Institute of Science Education and Research, Mohali. This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Wherever contributions of others are involved, every effort has been made to indicate that clearly. Due acknowledgement of collaborative research and discussions has been made. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Atul Singh Arora
(candidate)

In my capacity as the supervisor of the candidate's project work, I certify that the aforesaid statements by the candidate are true to the best of my knowledge.

Prof. Arvind
(supervisor)

Dated: April 22, 2016

Certificate of Examination

This is to certify that the dissertation titled **Contextuality in a Deterministic Quantum Theory**, submitted by **Mr. Atul Singh Arora** (Registration Number: MS11003) for the partial fulfilment of the BS-MS dual degree programme of the Indian Institute of Science Education and Research, Mohali, has been examined by the thesis committee duly appointed by the institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

Dr. Abhishek Chaudhuri	Dr. Kamal P. Singh	Prof. Arvind (supervisor)

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Abstract

The Copenhagen Interpretation of Quantum Mechanics (QM) asserts that the wavefunction is the most complete description, which entails that there is an inherent fuzziness in our description of nature. There exists a completion of QM, known as Bohmian Mechanics (BM), which replaces this fuzziness with precision, and re-introduces notions of physical trajectories. Various interesting questions arise, solely by the existence of such a description; doesn't it contradict the uncertainty principle, for instance. Most of these questions were found to have been addressed satisfactorily in the literature. There was, however, one question, whose answer has become the subject of the thesis; that of the paradoxical co-existence of contextuality and BM. In a theory that can predict the value of operators, the value an operator takes, must depend on the state of the system (including hidden variables). Contextuality arguments show that the value an operator takes, must also depend on the complete set of compatible operators, to be consistent with QM. BM being deterministic, is at complete odds with this notion.

After various attempts we were able to show, that the notion of contextuality is in fact not necessary. This was achieved by identifying another 'classical property' and constructing a non-contextual toy-model, serving as a counter-example to the impossibility proof. The toy model has been generalized to a discrete but arbitrarily sized Hilbert space, consistent with all predictions of QM. Implications of violation of this 'classical property' have been discussed, in particular, to the notion of non-locality.

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Prologue

1.1 Overview

A course in Quantum Mechanics (QM) typically leaves the reader with a fuzzy view of the world. The founders of the subject were able to abstract out the mathematics from its implications and interpretation. The view that the wavefunction is the most complete description of a system, known as the 'Orthodox Copenhagen Interpretation', is among the most popular. Einstein and Bohm, both played an important role in challenging this belief. Einstein showed [EPR35] that if one makes reasonable assumptions about nature (in the spirit of his relativity theories), then QM must be incomplete. By incompleteness, he meant that the results of certain experiments should be predictable precisely, but QM fails at doing this. Thus, he concluded that, QM must be treated as an intermediate theory and that a more complete description of nature should be sought. We will come back to this discussion.
Bohm challenged this view by realizing that one can't experimentally refute the interpretation. His argument was that if for instance, the predictions of QM fail to match with experiments, then one can always add appropriate terms in the Hamiltonian until the difficulty is resolved. He was already anticipating the modern form of particle physics. To accurately account for interactions between particles, one can postulate new force mediating particles, which was also done in the history of the subject. However, one can't refute the interpretation on grounds of inaccuracy in predictions. He, therefore, aimed at, and succeeded at constructing a complete quantum theory [Boh52a], now known as Bohmian Mechanics (BM)[1]. Its existence showed that we are not justified at believing the interpretation, simply because there exists at least one alternative.

Returning to Einstein, Bell was able to construct a physical situation, that would test the very requirements Einstein imposed on a complete quantum theory; he was able to show that according to predictions of QM, *such* a complete description is impossible. This

[1]Historically, Louis de Broglie had proposed a similar construction, but abandoned the idea soon after. Bohm established it to be a consistent theory.

was verified experimentally [FC72, AGR81] (and was confirmed to be true, without any possible loop-holes [HBD+15], only in 2015).
It might appear that Bell's test shows that QM is inconsistent with BM. Upon looking at the details however, one can be convinced, that this is not the case. In fact, Bell was among the first few to popularize BM [Bel04].

The discussion so far is well known in the literature. However, certain developments which followed the said work of Bohm, again lead to apparent inconsistencies between BM and QM. These had not been satisfactorily addressed in the literature and have become the subject of this thesis.
For the sake of completeness, we merely name these. One must look at the details, to be able to appreciate them. Greenberger, Horne and Zeilinger (GHZ), constructed a test [GHSZ90] that apparently showed determinism can't exist, i.e. the notion that observables have pre-defined values is inconsistent with QM. Developments due to Gleason [Gle57], Bell himself [Bel66], Kochen & Specker [KS67], and Peres & Mermin [Per91, Mer90] showed that the value an operator takes, must depend on the context in which it is measured; context here refers to the complete set of compatible operators.
The apparent contradiction must now be clear; BM is deterministic and it is at odds with the notion of contextuality as well.

1.2 The EPR argument

The EPR argument requires an entangled state, over two particles, which was originally written as

$$\psi(q_1,q_2)=\int e^{-i(q_1-q_2+q_0)p/\hbar}dp=\delta(q_1-q_2+q_0).$$

In the modern notation, one can write this as

$$\begin{aligned}|\psi\rangle &= \int \delta(q_1-q_2+q_0)dq_1dq_2\,|q_1\rangle_A\,|q_2\rangle_B\\ &= \int |q\rangle_A\,|q+q_0\rangle_B\,dq.\end{aligned}$$

Similarly, one can write the same state as

$$\begin{aligned}|\psi\rangle &= \int e^{-i(q_1-q_2)p/\hbar}dp\,dq_1dq_2\,|q_1\rangle_A\,|q_2\rangle_B\\ &= \int e^{-iq_1p/\hbar}\,|q_1\rangle_A\,dq_1 e^{iq_2p/\hbar}\,|q_2\rangle_B\,dq_2dp\\ &= \int |p\rangle_A\,|-p\rangle_B\,dp.\end{aligned}$$

where A and B label the particles. An attempt to reproduce the precise argument, will not be made. Instead, we satisfy ourselves with the following simplified argument. We assume the principle of locality holds, which is to say that if two particles are sufficiently far away, then any change made to one particle, should not influence the other instantaneously. Given this assumption, consider two particles, which are sufficiently far away and that their state is given by $|\psi\rangle$. Now if the momentum of particle B is measured by observer B, then observer B, according to QM, will be able to predict the momentum of particle A. Similarly, if the position of particle B is measured, then observer B can predict the position of particle A. Further, note that the choice made by observer B, can't influence particle A, by the assumption of locality. It therefore follows that particle A had both its position and momentum well defined, without being measured. QM fails to yield the answer with precision, whereas as we have shown, the answer was precise. Thus, we are forced to conclude that QM is not a complete description of nature.

Einstein ended his paper with this remark: "While we have thus shown that the wave function does not provide a complete description of the physical reality, we left open the question of whether or not such a description exists. We believe, however, that such a theory is possible." [EPR35]

1.3 Bell's Theorem

Bell's work addresses and satisfactorily answers Einstein's open question, of whether *such* a description exists. Consider the following scenario. There are two observers, A and B, each has a particle. Each observer, can measure two properties, call them $\hat{a}_1, \hat{a}_2$ for observer A and $\hat{b}_1, \hat{b}_2$ for observer B, which yield ± 1. Let $\langle \hat{a}_i \hat{b}_j \rangle$ represent the average value obtained by measuring the property $\hat{a}_i$ and $\hat{b}_j$ on the first and second particle respectively. Consider the average given by $\langle \hat{B} \rangle = \langle \hat{a}_1 \hat{b}_1 \rangle + \langle \hat{a}_1 \hat{b}_2 \rangle + \langle \hat{a}_2 \hat{b}_1 \rangle - \langle \hat{a}_2 \hat{b}_2 \rangle$. If one assumes local realism[2], that is that the values a_i takes are unaffected by those taken by b_i and that $\hat{a}_i, \hat{b}_j$ have pre-defined values (respectively), then $\langle \hat{B} \rangle \leq 2$. One can check this quickly by a brute force substitution of ± 1 values, in place of a_i, b_j.

Consider now, the state $|\psi\rangle = (|+-\rangle - |-+\rangle)/\sqrt{2}$, where $\hat{\sigma}_x |\pm\rangle = \pm |\pm\rangle$, and $\hat{\sigma}_{x,y,z}$ are the Pauli matrices, given in the z-basis as

$$\hat{\sigma}_x \doteq \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \hat{\sigma}_y \doteq \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \hat{\sigma}_z \doteq \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Let $\hat{a}_1 = \hat{\sigma}_z$ and $\hat{a}_2 = \hat{\sigma}_x$, while $\hat{b}_1 = -\frac{\hat{\sigma}_z + \hat{\sigma}_x}{\sqrt{2}}$ and $\hat{b}_2 = \frac{\hat{\sigma}_z - \hat{\sigma}_x}{\sqrt{2}}$. Upon evaluating $\langle \hat{B} \rangle$ using the rules of QM, one obtains $\langle \hat{B} \rangle = 2\sqrt{2} \nleq 2$. This entails that our assumption, that of local realism, must be incorrect, which settles the question: A *local* hidden variable description can not exist. The word hidden is used to represent information about the state of the system, that is not contained in the wavefunction. It is instructive to emphasize that a non-local description, may still be possible. It is also important to note that, despite this non-

[2] In fact, an argument similar to EPR can be used to show that locality entails realism.

locality, one can't use QM to send signals instantaneously (superluminal communication is not possible). This is known as the no-signalling theorem and can be proven by showing that marginals in QM, don't depend on the system which is traced out [NC11].

1.4 Bohm's Theory, Bohmian Mechanics (condensed introduction)

Bohm gave a precise [Boh52a], but non-local description of quantum phenomena. Let us start with non-interacting particles. A particle is associated with (1) a position, q & momentum, p, precisely defined and (2) a wavefunction $\psi = Re^{iS/\hbar}$. The postulates of the theory are: (a) Evolution of the wavefunction, is governed by Schrödinger's equation: $i\hbar\partial\psi/\partial t = -(\hbar^2/2m)\nabla^2\psi + V\psi$. (b) The particle is guided by the wavefunction: $\dot{q} = p/m$ where $p = \nabla S = \hbar\mathrm{Im}(\nabla\psi/\psi)$. (c) The initial distribution of the particles is given by $\rho(x) = |\psi|^2$.

The astute reader would've noticed that ∇S is just the probability current, which entails that if the initial distribution satisfies $|\psi(t_0)|^2$, then it will do so at all times t, thereafter. Before generalizing this to multiple particles, let us first see a quick consequence of this formulation. In the Orthodox Copenhagen interpretation, the double slit experiment is a source of mystery and the which slit question, that of confusion. In BM, since trajectories are well defined, one observes (see Figure 1.1) that the particle goes through precisely one slit and then later, forms the interference pattern. The wavefunction goes through both slits and interferes to create the pattern. If one of the slits is blocked, then since the wavefunction can't interfere, the pattern is lost as expected. We haven't spoken about measuring the particle yet, but if one notes that to measure the particle, the potential at one of the slits must be changed, then it is immediate that the interference pattern will be effected, since the wavefunction is affected by the potential at both slits, even if the particle passes through only one. One finds that by using the following multi-particle generalization, and an appropriate measuring scheme, one can show more precisely how the process of measuring effectively destroys the pattern, replacing the mystery with clarity.

For N interacting particles, we have $p_i = \nabla_i S(q_1, q_2, \ldots, q_N)$ where note that the momentum of the i^{th} particle, depends on the instantaneous positions of all the particles. Consequently, BM is an explicitly non-local, but complete description.

As a final remark, it must be added that spins can also be included in BM, however, a particle is not associated with a specific spin, only it's wavefunction is. For a spinor, say $\psi \equiv (\psi_+, \psi_-)^T$, the generalization is that $p = \hbar\mathrm{Im}((\psi, \nabla\psi)/(\psi, \psi))$ where $(.,.)$ represents inner product in the spin space $\mathbb{C}^2$. A quick illustration is in order. Consider the following Stern-Gerlach setup; Quantum effects are considered only along the x-axis. A particle moves along the z-axis, with speed v_z, and it's initial wavefunction, given by a Gaussian

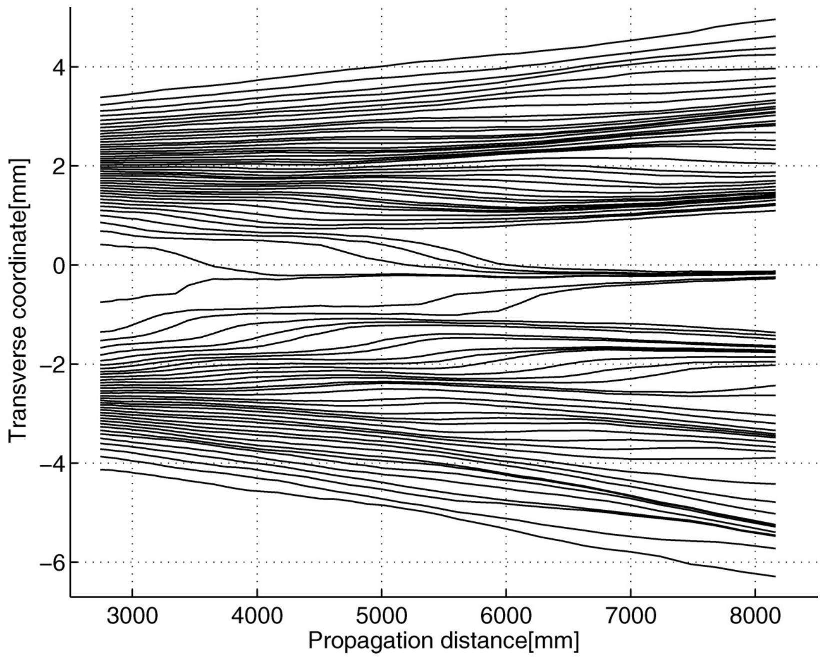


Figure 1.1: Experimentally observed average single-photon trajectories. "In the case of single-particle quantum mechanics, the trajectories measured in this fashion reproduce those predicted in the Bohm–de Broglie interpretation of quantum mechanics" [KBR+11]

centred at the origin, say $\psi(q_x) = (1/\sqrt{2\pi}\sigma)e^{-q_x^2/2\sigma^2}$, viz. $|\psi\rangle = \int dq\psi(q)|q\rangle$. It's spin state is given by $|\chi\rangle = (|+\rangle + |-\rangle)/\sqrt{2}$, where $|+\rangle$ and $|-\rangle$ are s.t. $\sigma_x|\pm\rangle = \pm|\pm\rangle$. Along the z-axis, a strong heterogeneous magnetic field is present, whose action maybe captured by $H_{\text{int}} = a\hat{p}_x \otimes \hat{\sigma}_x$ where a is a constant that quantifies the strength of the field. Why this particular form works, will become clear momentarily. Assuming that a is large enough to neglect effects of free-evolution, we have $\hat{U}(t) = e^{-ia\hat{p}_x\otimes\hat{\sigma}_x t/\hbar}$. Thus, if the initial state is $|\Psi\rangle = |\psi\rangle \otimes |\chi\rangle$, then

$$
\begin{aligned}
|\Psi(t)\rangle &= \hat{U}(t)|\Psi\rangle \\
&= \frac{e^{-ia\hat{p}_x t/\hbar}|\psi\rangle \otimes |+\rangle + e^{ia\hat{p}_x t/\hbar}|\psi\rangle \otimes |-\rangle}{\sqrt{2}} \\
&= \frac{|\psi_{at}\rangle \otimes |+\rangle + |\psi_{-at}\rangle \otimes |-\rangle}{\sqrt{2}}
\end{aligned}
$$

where $|\psi_{q_{x0}}\rangle \equiv \int dq\psi(q_x - q_{x0})|q_x\rangle$, viz. a Gaussian wavepacket centred at q_{x0}. One can plot $|\Psi|^2$, as a function of q_z, using $q_z = v_z t$, schematically as shown in the figure (see Figure 1.2), where regions enclosing, say 70% of $|\Psi(q_x)|^2$ have been outlined[3]. So far, according to QM, if we measure the position of the particle, then (given $\sigma \ll at$), obtaining the particle near $q_x = at$, is as probable as finding it near $q_x = -at$. QM doesn't make a deterministic prediction at this stage. According to BM, if in addition to the wavefunction, we assume that the particle was initially at some $q_x > 0$, then we can predict precisely where

[3]Note that $|\Psi|^2 = \langle\Psi|q_x\rangle\langle q_x|\Psi\rangle$, where the spins are essentially traced over by the said expression

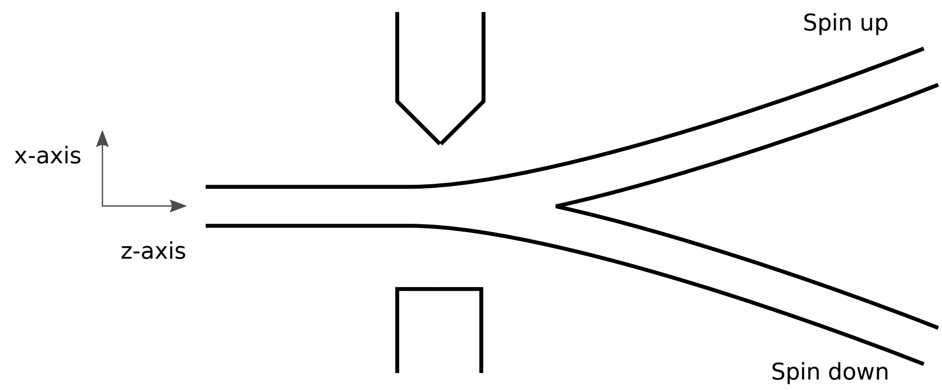


Figure 1.2: Contour plot of $|\Psi(q_x,t)|^2$ plotted for various $t = q_z/v_z$, illustrating a Stern-Gerlach measurement.

the particle will turn up. In fact, one can accomplish this with essentially no calculation. Since $\dot{q}_x = \nabla S/m$, a single-valued function, it follows that trajectories of particles won't intersect, where recall that S is given by $\psi = Re^{iS/\hbar}$. Consequently, a particle that starts with $q_x > 0$, must follow the 'up' trajectory, else by symmetry, the trajectories will have to intersect. We conclude, therefore, that if $q_x > 0$ initially, the particle has spin $|+\rangle$ and if $q_x < 0$, the spin must be $|-\rangle$. This appears very clear and intuitive. A non-intuitive aspect of this is that we can't associate spins with particles, even though we can predict precisely, the outcome of the experiment. This is manifested by the observation that if $H_{\text{int}} \to -H_{\text{int}}$, which practically amounts to reversing the heterogeneity of the magnet, then $\sqrt{2}|\Psi(t)\rangle = |\psi_{-at}\rangle \otimes |+\rangle + |\psi_{at}\rangle \otimes |-\rangle$. Again, if $q_x > 0$ initially for a particle, it will follow the 'up' trajectory. However, now this corresponds to spin $|-\rangle$, as opposed spin $|+\rangle$. We have thus demonstrated that we can't associate spin uniquely to a particle and that it must only be associated with the wavefunction [DT10].

As an aside, it may be added that BM is known for removing the fundamental role of an observer from the description of QM. This is accomplished, roughly speaking, by introducing the positions of particles as well defined, and then explaining the 'collapse' of wavefunction, by means of the particle's interaction with those in the environment, which entails that the 'collapsed wavefunction' serves as an effective wavefunction, which can be used to describe the motion of the particle henceforth [Boh52b, DT10].

1.5 Determinism: The GHZ test

One drawback of Bell's test was its statistical in nature. The GHZ test [GHSZ90], takes this a step further and shows that one can't even conceive of having pre-defined values. The construction requires three observers with one particle each. Each observer can measure two properties, X and Y, with outcomes ± 1. We start with the state $\sqrt{2}|\chi_G\rangle = |000\rangle - |111\rangle$ and note that for $\hat{A} := \hat{\sigma}_x \otimes \hat{\sigma}_y \otimes \hat{\sigma}_y$, $\hat{A}|\chi_G\rangle = |\chi_G\rangle$, where the property X is the projection of spin of the particle along the x-axis and Y is that along the y-axis. Thus a measurement of $\hat{A}$ (the first observer measures X and the other measure Y), will yield $+1$ with certainty. Next, we define $\hat{B} := \hat{\sigma}_y \otimes \hat{\sigma}_x \otimes \hat{\sigma}_y$ and $\hat{C} := \hat{\sigma}_y \otimes \hat{\sigma}_y \otimes \hat{\sigma}_z$, which by symmetry, must also yield $+1$ for the said state. If these observables, X and Y had predefined values, then a measurement of $\hat{A}\hat{B}\hat{C}$ would be equivalent to measuring $\hat{D} := \hat{\sigma}_x \otimes \hat{\sigma}_x \otimes \hat{\sigma}_x$, since Ys appear twice for each particle, and $Y^2 = 1$. Since a measurement of each $\hat{A}$, $\hat{B}$ and $\hat{C}$ yields a $+1$, it follows that a measurement of $\hat{D}$ therefore, must also yield $+1$. However, $\hat{D}|\chi_G\rangle = -|\chi_G\rangle$, which entails that a measurement of $\hat{D}$ must yield a -1. Thus, we arrive at a contradiction and conclude that the assumption that the properties X and Y had predefined values, must be incorrect. One could object that X and Y are complementary properties (correspond to non-commuting operators) and therefore it doesn't make sense to assign values to these operators and treat them like numbers. This objection is addressed by the contextuality tests.

1.6 Contextuality: The Peres Mermin test

There have been various developments, of which the simplest, with effectively the same consequence, is discussed: the Peres Mermin test [Per91, Mer90]. In this test also, we will show that pre-defined values can't exist, but in addition, also define the notion of contextuality. Consider the following set of operators

$$\hat{A}_{ij} \doteq \begin{bmatrix} \hat{\mathbb{I}} \otimes \hat{\sigma}_x & \hat{\sigma}_x \otimes \hat{\mathbb{I}} & \hat{\sigma}_x \otimes \hat{\sigma}_x \\ \hat{\sigma}_y \otimes \hat{\mathbb{I}} & \hat{\mathbb{I}} \otimes \hat{\sigma}_y & \hat{\sigma}_y \otimes \hat{\sigma}_y \\ \hat{\sigma}_y \otimes \hat{\sigma}_x & \hat{\sigma}_x \otimes \hat{\sigma}_y & \hat{\sigma}_z \otimes \hat{\sigma}_z \end{bmatrix}$$

which have the peculiar property that all operators along a row (and along a column) commute. It is trivial to see that this holds for the first two rows and the first two columns. To see that this holds also for the last row and column, note the anti-commutation relation, $\{\hat{\sigma}_x, \hat{\sigma}_y\} = 0$ and that $\sigma_z = i\sigma_y\sigma_x$, which one may check explicitly. Another interesting property is that the product of rows (columns) yield $\hat{R}_i = \mathbb{I}$ and $\hat{C}_j = \mathbb{I}\,(j \neq 3)$, $\hat{C}_3 = -\mathbb{I}$, $(\forall i, j)$ where $\hat{R}_i \equiv \prod_j \hat{A}_{ij}$, $\hat{C}_j \equiv \prod_i \hat{A}_{ij}$. This can be verified easily by using the aforesaid relations and the fact that $\sigma^2 = 1$, for every Pauli matrix. Using this property of R_i and C_j, it is easy to show that no pre-defined values for operators can exist. Let us assume that pre-defined values do exist. Note that to get $C_3 = -1$, we must have an odd number of -1 assignments in the third column. In the remaining columns, the number of -1 assignments must be even for each column. Thus, in the entire square, the number of -1 assignments must be odd. Let us use the same reasoning, but along the rows. Since each $R_i = 1$, we must have even number of -1 assignments along each row. Thus, in the entire square, the number of -1 assignments must be even. We have arrived at a contradiction and therefore we conclude that our assumption that operators have predefined values, must be wrong. One can in fact construct the following inequality

$$\langle\hat{\chi}_{\mathrm{PM}}\rangle = \langle\hat{R}_1\rangle + \langle\hat{R}_2\rangle + \langle\hat{R}_3\rangle + \langle\hat{C}_1\rangle + \langle\hat{C}_2\rangle - \langle\hat{C}_3\rangle \leq 4,$$

if it is assumed that operators have predefined values. This can be seen from an application of the aforesaid logic, which forbids an assignment that yields only one column (row) as -1. The next best assignment, viz. one that has two columns (or rows) set to -1, yields $\langle\hat{\chi}_{\mathrm{PM}}\rangle = 4$ at best. Of course, according to QM $\langle\hat{\chi}_{\mathrm{PM}}\rangle = 6 \nleq 4$, which is easier to verify experimentally. Thus a violation of the Peres Mermin inequality, again entails that our assumption is wrong. Note that unlike the GHZ test, the Peres Mermin test is (a) state independent (no specific $|\chi\rangle$ is needed for a violation) and (b) here, values of only commuting observables are multiplied.

We are now in a position to discuss the notion of contextuality. We begin with defining a non-contextual assignment to be one, where the assignment depends only on the state ($|\chi\rangle$ + hidden variables, if any) and the operator to which the assignment is being made. It follows that we had tacitly assumed a non-contextual assignment, that resulted in a contradiction. If we allow for the value of an operator, to depend on the context in which it is measured, where the context is meant to refer to a set of compatible observables, then the contradiction won't arise. For instance, if we imagine that all observables yield a $+1$, except $\hat{A}_{33}$ which yields a -1 if measured with $\hat{A}_{32},\hat{A}_{31}$ and yields a $+1$ if measured with $\hat{A}_{23},\hat{A}_{13}$. If this doesn't appear entirely unsatisfactory, then you're on the right track and are encouraged to read the more detailed description given in Chapter 4 (more specifically, Subsection 4.3.1).

Chapter 2

Determinism Tests and Bohmian Mechanics

2.1 Rationale

As was pointed out in the previous chapter, it is known that BM doesn't assign a unique value to the spin of a particle. For BM, spin is only a property of the wavefunction. Recall that the GHZ test was formulated for spins. Consequently, the conclusion that spins can't have pre-defined values (deterministic) does not contradict BM outright. Precisely how the GHZ test is compatible with BM, is worth exploring. It will edify our understanding of how to analyse a physical situation using BM and the relation between determinism & non-locality.

From the point of view of QM however, the treatment of spins is not fundamentally different from that of phase-space variables (position q and momentum p). It is not surprising, therefore, that the GHZ test can be generalized to phase space and at least one such extension is known [MP01]. The conclusion one draws from the phase space GHZ test, would then be that q, p can't have pre-defined values. This then is in direct contradiction with BM, which claims that q, p are precisely defined and their evolution completely determined (given the initial position, q_0, and the wavefunction). Since it is believed that BM is completely consistent with QM, it is of considerable interest to explore how BM can resolve the apparent paradox. If it fails, then we would have identified a way to falsify BM.

2.2 GHZ

For convenience, we recall that in our previous discussion, $\hat{A} \equiv \hat{\sigma}_x \otimes \hat{\sigma}_y \otimes \hat{\sigma}_y$, $\hat{B} \equiv \hat{\sigma}_y \otimes \hat{\sigma}_x \otimes \hat{\sigma}_y$, $\hat{C} \equiv \hat{\sigma}_y \otimes \hat{\sigma}_y \otimes \hat{\sigma}_x$, and $\hat{D} \equiv \hat{\sigma}_x \otimes \hat{\sigma}_x \otimes \hat{\sigma}_x$, which are such that $\hat{A}\,|\chi\rangle = \hat{B}\,|\chi\rangle = \hat{C}\,|\chi\rangle = |\chi\rangle$, while $\hat{D}\,|\chi\rangle = -\,|\chi\rangle$, for $\sqrt{2}\,|\chi\rangle = |000\rangle - |111\rangle$.

2.2.1 Compatibility with BM

To analyse any situation using BM, one is required to know the experimental arrangement. In this case, we assume that spins are measured using the Stern-Gerlach (SG) apparatus. Without loss of generality, let us assume that the initial state of the particle is given by, $\sqrt{2}|\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3,t=0)\rangle = |\psi_{+++}(\vec{r}_1,\vec{r}_2,\vec{r}_3,t=0)\rangle \otimes |000\rangle - |\psi_{---}(\vec{r}_1,\vec{r}_2,\vec{r}_3,t=0)\rangle \otimes |111\rangle$, where $\vec{r}_i$ represents the position vector in the frame of the i^{th} observer. Note that the explicit tensor product is used to separate the spin and position parts the three particles. If the wavefunction for each particle is assumed to be Gaussian initially, propagating along their respective axes of the SG apparatus, then one can further simplify the form of $|\psi_{\pm\pm\pm}\rangle$. It has been shown [DP02] that the time evolution of $|\psi_{\pm\pm\pm}\rangle$ can be written as products of 3 single particle solutions of the SG setup, which was analyzed by Bohm himself. Once $|\Psi(\vec{r}_i,t)\rangle$ is known, one can evaluate the equation of motion for the three particles, using BM. If the SG apparatus are setup to measure, say, XYY, then from both numerical simulations & analysis of the trajectory equations, the following is observed in the direction relevant to measurement. Four attractor basins are formed: $(+++)$, $(+--)$, $(-+-)$, and $(--+)$, where $\pm$ represent the physical location in the SG, corresponding to a spin 'up' ('down') measurement. The product is always $+1$, consistent with predictions of QM. However, when the SG apparatus are setup to measure XXX, the trajectories are found to obey equations which possess four attractive basins: $(---)$, $(-++)$, $(+-+)$ and $(++-)$. Again, the product is -1, in agreement with QM.

As a remark, it may be stated, that the details of evaluating the trajectory, become complicated rather quickly and that it is not trivial to obtain analytic solutions for the phase-space scenario. Consequently, numerical simulations are a necessity beyond this stage. (See [DP02] for a flavour of the complexity)

In conclusion, one finds that non-locality enters the description from the fact that the attractor basins which form, depend on the settings of *all* SG apparatus. Thus, we learn that while all the results are deterministic, they depend on the precise experimental setup, and not merely operators.

2.2.2 Phase Space

To extend the GHZ test to phase space, note first that we need only the following situation. Consider instead of observables (which are Hermitian), unitary operators, $\hat{X}$ and $\hat{Y}$ with the following redefinitions: $\hat{A} \equiv \hat{X}^\dagger \otimes \hat{Y} \otimes \hat{Y}^\dagger$, $\hat{B} \equiv \hat{Y}^\dagger \otimes \hat{X}^\dagger \otimes \hat{Y}$, $\hat{C} \equiv \hat{Y} \otimes \hat{Y}^\dagger \otimes \hat{X}^\dagger$ and $\hat{D} = \hat{X} \otimes \hat{X} \otimes \hat{X}$. If these unitary operators also satisfy $\{\hat{X},\hat{Y}\} = 0 = \{\hat{X},\hat{Y}^\dagger\}$, then it follows that (a) $\hat{A}$, $\hat{B}$, $\hat{C}$ and $\hat{D}$ all commute and (b) $\hat{A}\hat{B}\hat{C}\hat{D} = -\mathbb{I}$. Now any simultaneous eigenket of $\hat{A}$, $\hat{B}$, $\hat{C}$ and $\hat{D}$ will yield a GHZ situation.

To see why that will work, replace the unitary operators with complex numbers and note that the unitary property translates to each of these numbers being uni-modular. Thus,

$ABC = X^* \otimes X^* \otimes X^*$, using $Y^*Y = 1$ for each particle. This would entail that $ABC = D^*$, viz. $ABCD = 1$. However we also know that $ABCD = -1$, which yields the contradiction.

Another patent issue with this scheme, is the use of unitary operators, as opposed to observables. This issue is resolved by explicit construction, however the idea can be motivated in general. If an arbitrary unitary operator, is a function of some fixed observable, and that alone, then one can measure the said observable. From this, the value of the unitary operator can be evaluated, thereby dissolving the objection.

2.2.2.1 Known Extension

One possible construction [MP01], involves the use appropriate displacement operators. $\hat{X} \equiv e^{i\sqrt{\pi}\hat{q}/L}$ and $\hat{Y} \equiv e^{i\sqrt{\pi}\hat{p}L}$, where L is some length scale and units are s.t. $\hbar = 1$ (for this section). These satisfy $\{\hat{X}, \hat{Y}\} = 0$, which follows trivially by recalling that $e^{i\hat{p}u}e^{i\hat{q}v} = e^{i\overset{1}{\hbar}uv}e^{i\hat{q}v}e^{i\hat{p}u}$. To construct a simultaneous eigenstate, observe that for

$$
\begin{aligned}
\sqrt{2}\left|\uparrow\right\rangle_{q_0,p_0} &\equiv \sum_{k=-\infty}^{\infty} e^{i\sqrt{\pi}2kp_0L}\left|q = \sqrt{\pi}L(q_0+2k)\right\rangle \\
&\quad + i\sum_{k=-\infty}^{\infty} e^{i\sqrt{\pi}(2k+1)p_0L}\left|q = \sqrt{\pi}L(q_0+2k+1)\right\rangle, \\
\sqrt{2}\left|\downarrow\right\rangle_{q_0,p_0} &\equiv \sum_{k=-\infty}^{\infty} e^{i\sqrt{\pi}2kp_0L}\left|q = \sqrt{\pi}L(q_0+2k)\right\rangle \\
&\quad - i\sum_{k=-\infty}^{\infty} e^{i\sqrt{\pi}(2k+1)p_0L}\left|q = \sqrt{\pi}L(q_0+2k+1)\right\rangle,
\end{aligned}
$$

where $p_0L/\sqrt{\pi}$ & $\sqrt{\pi}Lq_0 \in [0,1)$, $\hat{X}\left|\uparrow\right\rangle = \left|\downarrow\right\rangle$, $\hat{Y}\left|\uparrow\right\rangle = i\left|\downarrow\right\rangle$ and similarly $\hat{X}\left|\downarrow\right\rangle = \left|\uparrow\right\rangle$, $\hat{Y}\left|\downarrow\right\rangle = -i\left|\uparrow\right\rangle$ (we have dropped q_0 and p_0 for simplicity). This also holds for $\hat{X}^\dagger$ and $\hat{Y}^\dagger$. To see this, note that $\hat{Y}^\dagger\left|q\right\rangle = \left|q+\sqrt{\pi}L\right\rangle$ while $\hat{X}\left|x\right\rangle = e^{i\sqrt{\pi}q/L}\left|q\right\rangle$. If one defines $\hat{Z} = i\hat{Y}\hat{X}$, from the aforesaid, it follows $\hat{Z}\left|\uparrow\right\rangle = \left|\uparrow\right\rangle$ and $\hat{Z}\left|\downarrow\right\rangle = -\left|\downarrow\right\rangle$. The problem has been made sufficiently analogous to the original GHZ test. It is now immediate that the required simultaneous entangled eigenket must be

$$
\left|\psi\right\rangle = \frac{\left|\uparrow\uparrow\uparrow\right\rangle - \left|\downarrow\downarrow\downarrow\right\rangle}{\sqrt{2}}.
$$

It is obvious that for obtaining the value of $\hat{X}$, one need only measure $\hat{q}$ and $\hat{p}$ to obtain the value of $\hat{Y}$ and their conjugates. We have therefore an extension of the GHZ test to continuous variables. To understand how BM explains this, however, one must be able to simulate this. The test in the given form is not simple to simulate since the states involved have infinite spread in position space (in fact one can show that even in momentum space the spread is infinite). Further, the wavefunction in position space is a countable union of disjoint delta functions. Neither of these is desired from the numerical point of view. The

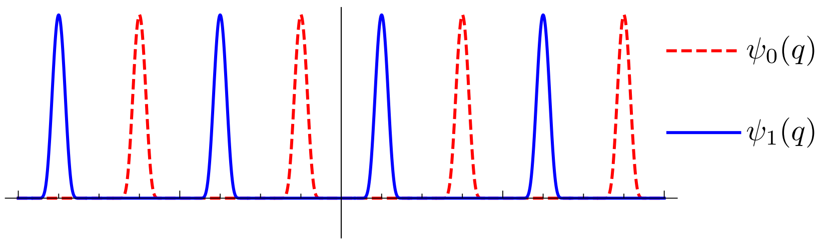


Figure 2.1: Illustration of multicomponent superposition states $|\psi_0\rangle$ and $|\psi_1\rangle$ for $N=8$ [AA15], used in the optimization of the GHZ test.

latter can be handled by integrating $|\uparrow\rangle_{q_0,p_0}$ over q_0 with an appropriate weight. However, no simple way could be conceived of to suppress the infinite spread.

2.2.2.2 Optimized Extension

This result was obtained after considerable effort. We construct an optimization of the phase space GHZ test, such that (a) the wavefunctions aren't sharp (no delta functions) and (b) that they disappear as $q\to\pm\infty$. We consider the same states $|\psi_0\rangle, |\psi_1\rangle$ for $N=2M=8$, as those considered in [AA15]. These are given by

$$|\psi_0\rangle \equiv \frac{1}{\sqrt{M}}\sum_{n=-\lfloor\frac{M}{2}\rfloor}^{\lfloor\frac{M-1}{2}\rfloor}|\varphi_{2n+1}\rangle\,, |\psi_1\rangle \equiv \frac{1}{\sqrt{M}}\sum_{n=-\lfloor\frac{M}{2}\rfloor}^{\lfloor\frac{M-1}{2}\rfloor}|\varphi_{2n}\rangle\,,$$

where $\varphi(q)=\langle q|\varphi\rangle$ is a localized state, symmetric about $q=L/2$, where L is some length scale and $\varphi_n(q)\equiv\varphi(q-nL)$ and M characterizes the 'size' of the state (see Figure 2.1). For $\hat{Z}\equiv Z(\hat{q})=\mathrm{sgn}(\sin(\hat{q}\pi/L))$, we have $\hat{Z}|\psi_0\rangle=|\psi_0\rangle$ and $\hat{Z}|\psi_1\rangle=-|\psi_1\rangle$. In addition to this, we define $\hat{X}=e^{-i\hat{p}L/\hbar}$ (note that this is not Hermitian). Observe that $|\psi_\pm\rangle\equiv\frac{|\psi_0\rangle+|\psi_1\rangle}{\sqrt{2}}$ is not an eigenstate of $\hat{X}$, although it comes close. We optimize the observable $\hat{X}$ to $\hat{X}'\equiv\hat{X}\hat{T}$, where $\hat{T}\equiv e^{i\hat{p}NLa(\hat{q})/2}$ and

$$a(q)=\begin{cases}1 & 2L<q<4L\\ 0 & \text{else}\end{cases}.$$

The idea is that you shift certain peaks to the right place, before applying the displacement operator $\hat{X}$. To illustrate this, consider explicitly $|\psi_0\rangle=(|\varphi_{-4}\rangle+|\varphi_{-2}\rangle+|\varphi_{-1}\rangle+|\varphi_{-3}\rangle)/\sqrt{4}$. The operation of $\hat{T}$ is $\hat{T}|\varphi_4\rangle=|\varphi_{-5}\rangle$, $\hat{T}|\varphi_3\rangle=|\varphi_{-6}\rangle$ and $\hat{T}|\varphi_n\rangle=|\varphi_n\rangle$ for $n\in\{-4,-3,-2,-1,1,2\}$. It is now evident that $\hat{X}'=\hat{X}\hat{T}|\psi_0\rangle=|\psi_1\rangle$. Note also that $\hat{X}'^\dagger|\psi_0\rangle=|\psi_1\rangle$. Similarly $\hat{X}'|\psi_1\rangle=|\psi_0\rangle$ and $\hat{X}'^\dagger$ does the same. So finally, consider $|\psi_G\rangle\equiv(|\psi_0\psi_0\psi_0\rangle-|\psi_1\psi_1\psi_1\rangle)/\sqrt{2}$. With $\hat{A}\equiv\hat{X}'\otimes\hat{Y}'\otimes\hat{Y}'^\dagger$, where $\hat{Y}'\equiv i\hat{Z}\hat{X}'$, calculations yield $\hat{A}|\psi_G\rangle=|\psi_G\rangle$. With $\hat{B}\equiv\hat{Y}'^\dagger\otimes\hat{X}'\otimes\hat{Y}'$ and $\hat{C}\equiv\hat{Y}'\otimes\hat{Y}'^\dagger\otimes\hat{X}'$ also, by symmetry we get $\hat{B}|\psi_G\rangle=|\psi_G\rangle$ and $\hat{C}|\psi_G\rangle=|\psi_G\rangle$. Now $\hat{E}\equiv\hat{A}\hat{B}\hat{C}=\hat{X}'\otimes\hat{Y}'\hat{X}\hat{Y}'^\dagger\otimes\hat{X}'$ and $\hat{D}\equiv\hat{X}'\otimes\hat{X}'\otimes\hat{X}'$ yield the paradox. If values were predefined, the value of $\hat{D}$ and $\hat{E}$ would return the same answer. However, a simple calculation yields $\hat{E}|\psi_G\rangle=|\psi_G\rangle$ (this can be seen directly by applying $\hat{A}$, $\hat{B}$ and $\hat{C}$ sequentially on $|\psi_G\rangle$), while $\hat{D}|\psi_G\rangle = -|\psi_G\rangle$.

The wavefunction now satisfies both the conditions required. The cost that one pays, however, is that a simple measurement of $\hat{q}$ and $\hat{p}$ won't suffice. It remains to see precisely which observable one must measure and what must be the analogue of the SG apparatus.

2.3 BM Simulator

Simulation of BM is a two step process. First, one must be able to simulate QM, viz. the Schrödinger equation and second, be able to evaluate the position of the particle at each time step.

2.3.1 Design of Numerics

The code was written in Fortran, due to its efficacy at handling arrays, in conjunction with gnuplot. Runge Kutta 4 was used to solve the differential equations and spline interpolation was used for calculating velocities of the particle. The initial goal was simply to find the trajectories for a single particle, with only one degree of freedom.

2.3.1.1 Simulation of Schrödinger's Equation

To simulate a differential equation, say $\dot{q} = f(q)$, one obvious method is to simply use $q_{n+1} = q_n + f(q_n)\Delta t$, $t_{n+1} = t_n + \Delta t$ where n parametrizes the sequence and Δt, the time step. To get reasonably accurate results, one needs to keep Δt small. This is known as the Euler method and it has errors of $\mathscr{O}(\Delta t^2)$. However, there's another known method, popularly referred to as "RK4", short for Runge Kutta 4, which has errors of $\mathscr{O}(\Delta t^5)$. Assuming again that $\dot{q} = f(q)$, the method claims that $q_{n+1} = q_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$, $t_{n+1} = t_n + h$, where

$$\begin{aligned}
k_1 &= f(q_n), \\
k_2 &= f(q_n + hk_1/2), \\
k_3 &= f(q_n + hk_2/2), \\
k_4 &= f(q_n + hk_3),
\end{aligned}$$

and $h = \Delta t$. The derivation is tangential to our interest and will have to be skipped. The advantage is that this method can produce accurate results for relatively larger Δt also.

Our purpose is to solve the Schrödinger Equation, viz. $\partial\psi/\partial t = -(\hbar^2/2m)(\partial^2\psi/\partial q^2) + V(q)\psi$. Clearly this is more complicated than the case discussed before, for now we have to solve for ψ, and ψ is a function of both q and t. We begin with uniformly discritizing ψ in the position space, so that ψ is known only at finite points $\{q_n\}$ to start with (and has spacing Δq), while time is discritized as usual, with step Δt. Imagine that we are at the n^{th} step, q_i and t_n are known, and so is $\psi_n(\{q_i\})$ (where the notation means that at the n^{th} step, ψ_n is known at all the points $\{q_i\}$). Given $\psi_n(\{q_i\})$, one can evaluate $\partial^2\psi/\partial q^2 = \psi''$ using the definition of the derivitive, without imposing the $h \to 0$ limit (in the usual notation) and obtain $\psi''(q_i) = [\psi(q_{i+1}) - 2\psi(q_i) + \psi(q_{i-1})]/(\Delta q)^2$. The objective is to find $\psi_{n+1}(q_i)$, which according to the Euler method can be evaluated as $\psi_{n+1}(q_i) = [-\psi''(q_i) + V(q_i)\psi]\Delta t$, where for illustration, we have set $\hbar^2/2m = 1$. Practically this doesn't suffice and we are forced to use RK4 (or any better alternative). To use RK4, one must be careful and remember that we are evaluating ψ for a given value q_i. Therefore in the evaluations of k_i, q_i must be kept fixed, for here ψ is the variable, playing the role of q. Ofcourse, ψ is a complex variable Accordingly, we must have, suppressing q_i to avoid confusion, $\psi_{n+1} = \psi_n + \frac{h}{6}(k_1 + k_2 + k_3 + k_4)$, where

$$
\begin{aligned}
k_1 &= -\psi_n'' + V\psi_n, \\
k_2 &= -(\psi_n + hk_1/2)'' + V(\psi_n + hk_1/2), \\
k_3 &= -(\psi_n + hk_2/2)'' + V(\psi_n + hk_2/2), \\
k_4 &= -(\psi_n + hk_3)'' + V(\psi_n + hk_3),
\end{aligned}
$$

and $h = \Delta t$. Let us take a moment to understand how one must go about evaluating this numerically. Since $\psi_n''(q_i)$ and $\psi_n(q_i)$ are known, one can evaluate $k_1(q_i)$ trivially. To evaluate $k_2(q_i)$ however, we would require $k_1(\{q_i\})$ to be known (or at least $k_1(q_{i-1})$, $k_1(q_i)$ and $k_1(q_{i+1})$). Thus, we first evaluate k_1 $\forall q_i$ in the grid. Then to evaluate $k_2(q_i)$, we need $(\psi_n + hk_1/2)''$, evaluated at q_i. Since the finite difference method requires it's argument to be known at q_{i-1}, q_i and q_{i+1}, we see that knowing $k_1(\{q_i\})$ is sufficient to evaluate this step. One similarly evaluates $k_2(\{q_i\})$ to evaluate $k_3(\{q_i\})$ and then $k_4(\{q_i\})$. It maybe added as remark, that practically it is found, that $\Delta t/\Delta x^2 \leq 10^{-6}$ or so for Euler and 10^{-4} or so for RK4, as was also pointed out by [JCT]. The aforesaid was observed to successfully simulate the Schrödinger equation, for a variety of potentials, details of which follow.

2.3.1.2 Simulation of trajectories

According to Bohmian Mechanics, $\dot{q} = p/m = \nabla S/m = \hbar \mathrm{Im}(\nabla\psi/\psi)$, where $\psi = Re^{iS/\hbar}$. From the previous section, we have ψ_n, discretized ψ at each time step. We conclude, therefore, that the simplest way to obtain ∇S at an arbitrary position, is to interpolate ψ and subsequently evaluate ∇S. Spline interpolation is quite standard and fairly simple to extend to complex variables. The details will not be discussed here, but the code written [see Subsection 2.3.3] can be referred to. It may be mentioned that given $\psi(\{q_i\})$, one can evaluate spline coefficients, using which, one can easily (in a computationally cheap way) evaluate $\psi(q)$ for practically any value of q. To evolve q, viz. to obtain q_n, again RK4 was used where this time, there are no complications. To be able to better appreciate the results, one needs to plot multiple trajectories simultaneously. The mildly non-trivial

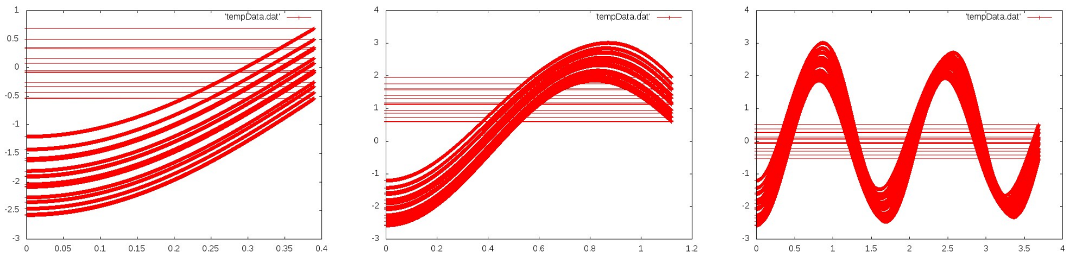


Figure 2.2: Simulated Bohmian trajectories for a harmonic oscillator.

aspect of this part is that one needs to start with particles distributed according to $|\psi|^2$. Attempts were made to find a library that can do this, but with no luck. A method to convert a uniform random distribution to an arbitrary distribution was independently arrived at, for a course on Numerical Methods. The idea was to use a uniform random generator, with range $[0,1]$, which for the j^{th} particle, yields $c^{(j)}$, say. The method is that, from the cumulative $\phi(q) = \int_{-\infty}^{q} |\psi(q')|^2 dq'$, one finds $q^{(j)}$ s.t. $\phi(q^{(j)}) = c^{(j)}$, viz. $q^{(j)} = \phi^{-1}(c)$. The inverse is guaranteed to be single valued because the cumulative is monotonically increasing. While a formal proof can be presented, we will satisfy ourselves with noting the following. Intuitively, a range of positions with high probability will cause a larger range of c values to yield those positions, making them more likely to appear; since all values of c are equally likely. With all these ingredients combined, Bohmian trajectories were successfully simulated.

2.3.2 Performance against analytic results

Three known physical situations were tested. (a) $V = 0$; It is known that a Guassian under free evolution, simply expands. (b) $V = \frac{1}{2}\omega^2 q^2$; It is known that a displaced Gaussian, oscillates under a harmonic potential (see Figure 2.2), and so does it's spread (unless a coherent state is chosen). (c) Double slit; By using a time varying potential, s.t.

$$V = \begin{cases} 0 & t \leq t_a \\ V_{\text{dw}} & t_a < t \leq t_b \\ 0 & t_b < t \end{cases}$$

where $V_{\text{dw}}(q)$ represents two wells, simulating the double slit effect, with a single degree of freedom.

In all cases, the results were qualitatively found to match. In the case of the double slit, although the wavefunction interference pattern was distorted, one could see the particles preferentially collecting at the maxima.

2.3.3 Simulation Results

BM was successfully simulated for a particle, with a single degree of freedom, influenced by an arbitrary potential. Implementing RK4, interpolation, and random distribution generation were among the non-trivial aspects. Generalization to multiple particles and inclusion of spins was among the immediate next steps, however due to later theoretical developments, were not carried out. The code is available at [Aro]

2.4 Measurements in BM (I)

Measurement of spins in BM was discussed in the previous chapter. Our interest in this chapter is in measuring q, p and functions thereof. We will learn that one can infact construct a universal method that facilitates the measurement of any arbitrary observable. The analysis will clarify two notions which are at high risk of being misconstrued. First, that the position of the particle, when measured, will infact yield q. However, a measurement of momentum of a particle, as we will see, does not always yield p (the value it had prior to measurement). In fact, it would be inconsistent with QM if it did; for instance, consider $\psi(q) = \left(1/\sqrt{\pi}\right) e^{-q^2}$, for which $S = 0$ and therefore so is $p = \nabla S = 0$. However, it is known that upon measurement of momentum, one obtains a distribution given by the Fourier transform of ψ. Although this is centred around the origin, it is not a delta function (has non-zero spread). The second notion which is clarified is that to find the value obtained upon measurement of certain observables, knowledge about the precise position of the measuring particle (the particle used to make the measurement) can play a deciding role.

2.4.1 Observable with discrete spectrum | Hamiltonian Approach

Bohm has discussed in his second paper [Boh52b], how any arbitrary observable may be measured, in BM. To describe a measurement, we use a measuring particle (mass m_L, say), by getting it to interact with the system for a short duration appropriately. Subsequently, we measure the final position of the particle, to learn about the value of the observable of interest. Say for instance, we wish to measure the observable $\hat{L}$, then the required interaction Hamiltonian is given by $\hat{H}_{\text{int}} = a\hat{L} \otimes \hat{p}$. Here the first operator acts on the system and second (after the tensor product symbol) acts on the measuring particle. a quantifies the interaction strength. It has dimensions of frequency, if L has dimensions of length. Let us assume that the system in the state $|\psi\rangle$. Then it is known that one can express $|\psi\rangle = \sum_l \langle l|\psi\rangle |l\rangle$, where $|l\rangle$ are the eigenstates of $\hat{L}$ with eigenvalue l (we have assumed non-degenercy for simplicity, but its removal doesn't cause any significant difficulty). $|\Psi_S(t)\rangle = \hat{U}(t) |\psi\rangle \otimes$

$|\varphi\rangle$, where

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\left[-\hbar^2\frac{\nabla_1^2}{2m}-\hbar^2\frac{\nabla_2^2}{2m_L}+\hat{H}_{\rm int}\right]t}$$

and $|\varphi\rangle$ is the state of the measuring particle, given by a Guassian centred at the origin, $\varphi(q) = (1/\sqrt{2\pi}\sigma)e^{-q^2/2\sigma^2}$. If t is very small, and a very large, s.t. $at = \lambda$ is a finite number, then one can neglect the free evolution, $\nabla^2 t$ terms compared to $\hat{H}_{\rm int}t$. We then have

$$\begin{aligned}
|\Psi_S(t)\rangle &= e^{-\frac{i}{\hbar}a\hat{L}\otimes\hat{p}t}\,|\Psi_S\rangle \\
&= \sum_l \langle l|\psi\rangle\,|l\rangle\otimes e^{-\frac{i}{\hbar}\lambda l\,\hat{p}}\,|\varphi\rangle \\
&= \sum_l \langle l|\psi\rangle\,|l\rangle\otimes|\varphi_{\lambda l}\rangle\,,
\end{aligned}$$

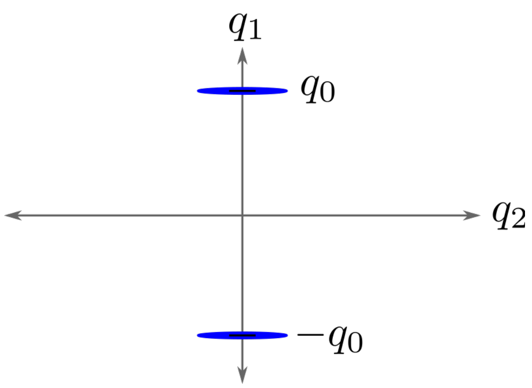
where $\left|\varphi_{q_0}\right\rangle = \int dq\varphi(q-q_0)\,|q\rangle$. This interaction, effectively entangles the measuring particle, with the possible 'outcomes', eigenstates of the observable $\hat{L}$ of interest. If $\sigma \ll \lambda l$, then according to QM itself, a position measurement of the measuring particle, would correspond, in a one-to-one way, to the eigenstate/eigenvalue of $\hat{L}$, to which the system will collapse. In the context of BM, after the interaction, the measuring particle would be guided into one of these eigenstates, and a position measurement would yield the same. We glossed over various details in making the last statement, which will be delineated shortly, through some illustrations.

2.4.1.1 Generalization to observables with continuum spectrum

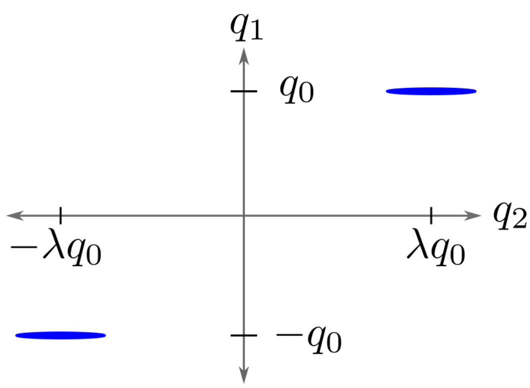
Since we are interested in observing phase space variables, the aforesaid must be generalized to the continuous spectrum regime. We proceed with the aforesaid notation and promote the discrete operator $\hat{L}$ to have a continuous spectrum. Thus $|\psi\rangle = \int dl\,\langle l|\psi\rangle\,|l\rangle$, and recall $|\varphi\rangle = \int dq\varphi(q)\,|q\rangle$, where $\varphi(q)$ has σ quantifying the deviation from the origin. Now $|\Psi_S(t)\rangle = \hat{U}(t)\,|\psi\rangle\otimes|\varphi\rangle = \int\int dldq\varphi(q)\,\langle l|\psi\rangle\,|l\rangle\otimes|q+l\lambda\rangle$, where $\lambda = at$ as before. Say q is measured at this stage and q' is the value obtained. The resultant state would then be $|q'\rangle\,\langle q'|\,|\Psi_S\rangle = \int\int dldq\varphi(q-l\lambda)\,\langle l|\psi\rangle\,|l\rangle\,\delta(q-q') = \int dl\varphi(q'-l\lambda)\,\langle l|\psi\rangle\,|l\rangle$. We know that $\varphi(q)\approx 0$ when $q\notin(-\delta q,\delta q)$, where $\delta q = \mathscr{O}(\sigma)$ can be chosen, depending on the accuracy desired. This implies $-\delta q < q'-l\lambda < \delta q$, which entails that $l = \frac{q'}{\lambda}\pm\frac{\delta q}{\lambda}$. We thus have a relation between the observed position, q', of the measuring particle, and the value of the operator $\hat{L}$. The error is controlled by the sharpness of the initial state of the measuring particle.

2.4.1.2 Consistency check; measurement of position

The position of a particle, as is claimed by BM, remains the same upon observing. Let us verify this statement, by applying the aforesaid formalism. For simplicity, let us assume that the state of the system is given as $\sqrt{2}\,|\psi\rangle = \int dq\,[\delta(q-q_0)+\delta(q+q_0)]\,|q\rangle$, which



(a) Before interaction



(b) After interaction

Figure 2.3: Indicative contour plot of $|\langle q_1,q_2|\Psi_S\rangle|^2$, illustrating consistency of position measurements.

is to say, the system is in a superposition of being at q_0 and $-q_0$. Let us assume that the particle is initially given to be in $q_1 = q_0$. Now our measurement formalism must be consistent with this, viz. the answer must not depend on the initial position of the measuring particle. Initially then, the state is $|\Psi_S\rangle = |\psi\rangle \otimes |\varphi\rangle$, while after interaction, the state becomes $\sqrt{2}|\Psi_S(t)\rangle = |q_0\rangle \otimes \left|\varphi_{\lambda q_0}\right\rangle + |-q_0\rangle \otimes \left|\varphi_{-\lambda q_0}\right\rangle$. To understand this clearly, one must plot $|\Psi_S(q_1,q_2)|^2 = |\langle q_1,q_2|\Psi_S\rangle|^2$, where $|q_1\rangle$ is (the position eigenket) for the system and $|q_2\rangle$ for the measuring particle. Before the interaction (see Figure 2.3a), say the measuring particle was at $q_2 \in (-\sigma,\sigma)$. After the interaction (see Figure 2.3b), the measuring particle will move to $q_2 \in (\lambda q_0 - \sigma, \lambda q_0 + \sigma)$, which follows simply by noting that the velocities are given by probability current. A measurement of the particle's position would yield $q_2 \approx \lambda q_0$, which we know from our analysis, corresponds to $q_1 = q_0$, which is in fact consistent with our initial conditions. It must be emphasized that the position of the measuring particle, plays no essential role in deciding where it would show up. The same analysis can be repeated for $q_1 = -q_0$ and in this case, from Figure 2.3b, it would follow that after the interaction, $q_2 \approx -\lambda q_0$. The consistency of this method is therefore established. Of course, one can relax the idealized δ functions to obtain more realistic functions, but the conclusion remains invariant.

2.4.1.3 Consistency check; measurement of momentum

We now resolve the issue pointed out in the beginning of this section, viz. the observed value of p being inconsistent with QM. We begin with writing the state of the system as $|\psi\rangle = \int dq \left(1/\sqrt{\pi}\right) e^{-q^2} |q\rangle$, so that $p = \nabla S = 0$. We wish to find, how the spread in the observed value of p appears, from the aforesaid measurement formalism. Note that

$$
\begin{aligned}
|\psi\rangle &= \int dp\,|p\rangle \int dq \overbrace{\langle p|q\rangle}^{\left(1/\sqrt{2\pi\hbar}\right) e^{-iqp/\hbar}} \psi(q) \\
&= \int dp \tilde{\psi}(p)\,|p\rangle\,,
\end{aligned}
$$

where $\tilde{\psi}(p)$ is $\psi(q)$ fourier transformed. The combined state before measurement is given by $|\Psi_S\rangle = |\psi\rangle \otimes |\varphi\rangle$, while after the measurement, $|\Psi(t)\rangle = \int dp \tilde{\psi}(p)\,|p\rangle \otimes |\varphi_{\lambda p}\rangle$. The aforesaid expression entails that, assuming $\sigma \to 0$, the probability for the measuring particle, to end up at λp, is given by $|\tilde{\psi}(p)|^2$, which is consistent with QM. To obtain this result more carefully from Bohmian trajectories, one must plot $|\langle q_1, q_2|\Psi_S\rangle|^2$ as was done in the previous section, but we will satisfy ourselves here, with noting that the measurement process has explicitly imparted momentum on the system, as is clear after 'collapsing' the wavefunction.

2.4.2 Classical limit of measurements

Although we have not yet discussed the classical limit of BM, as an aside, it may be demonstrated that this indeed follows elegantly. If we write $\psi = Re^{iS/\hbar}$ and substitute this in the Schrödinger Equation, and separate the real and imaginary parts, we obtain

$$
\begin{aligned}
\frac{\partial R}{\partial t} &= -\frac{1}{2m}\left[R\nabla^2 S + 2\nabla R.\nabla S\right], \\
\frac{\partial S}{\partial t} &= -\left[\frac{\nabla S^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}\right].
\end{aligned}
$$

The reader would've recognized that the second equation is essentially the Hamilton Jacobi equation, with an extra term. Infact, if one writes $P = R^2$, then we obtain

$$
\begin{aligned}
\frac{\partial P}{\partial t} + \nabla.\left(P\frac{\nabla S}{m}\right) &= 0 \\
\frac{\partial S}{\partial t} + \frac{\nabla S^2}{2m} + V - \frac{\hbar^2}{4m}\left[\frac{\nabla^2 P}{P} - \frac{1}{2}\frac{\nabla P^2}{P^2}\right] &= 0
\end{aligned}
$$

which makes the first equation effectively a continuity equation for probabilities, if one relates $\nabla S = p$ (momentum in BM), as is done in the Hamilton Jacobi framework. Effectively then, BM elegantly yields the classical limit, for if we neglect the $\hbar$ term, then we have particles obeying Newton's laws.

Our motivation was to study how the measured value of momentum turns out to be $p = \nabla S$ in the classical limit. The larger goal was to use this elegant framework, to understand how measurement of functions of q, p, such as the energy, for example, become equivalent to measuring q and p and plugging their values into the function. To be precise, consider the example of an energy eigenstate in a harmonic potential. For this state, neither q nor

p are precisely defined (in the language of QM), however, the energy is sharp. We started with analysing the classical limit of the measurement process, just discussed. That requires the potential V, to be a function of both q and p, whereas for the aforesaid derivation, only position dependent V was used. Correcting for this, create various issues. First of all, this interaction adds a term to the continuity equation,

$$\frac{\partial P}{\partial t}+\nabla_1\left(P\frac{\nabla_1 S}{m}\right)+\nabla_2\left(P\frac{\nabla_2 S}{m}\right)+\overbrace{2aR\left[\nabla_1 R\nabla_2 S+R\nabla_1\nabla_2 S+\nabla_2 R\nabla_1 S\right]}^{\text{Extra Term! | How will } P \text{ satisfy the continuity equation?}}=0.$$

The interaction also adds a "quantum potential" in addition to the expected potential, which doesn't seem to disappear in the large mass limit,

$$\frac{\partial S}{\partial t}+\frac{(\nabla_1 S)^2}{2m}+\frac{(\nabla_2 S)^2}{2m}+\overbrace{a\nabla_1 S\nabla_2 S}^{\text{expected part}}-\overbrace{a\hbar^2\frac{\nabla_1\nabla_2 R}{R}}^{\text{quantum part}}-\underbrace{\frac{\hbar}{2mR}(\nabla_1^2 R+\nabla_2^2 R)}_{\text{usual quantum potential}}=0.$$

One can see that with $\hbar\to 0$, the quantum potential and the quantum part of the interaction, both disappear. However, the continuity equation is not recovered still. This part was not explored further, but can perhaps be studied independently of our current target.

2.4.3 Measurement Exploration Summarized

From the optimized GHZ construction, it was necessary to arrive at a theoretical construction, that would allow calculation of measurement outcomes associated with arbitrary operators composed using $\hat{q}$, $\hat{p}$. This was achieved, however, it was found that obtaining these results is not trivial in most cases of interest. The surprising result, that measurement of $\hat{p}$ may not yield $p=\nabla S$, while a measurement of $\hat{q}$ yields q, was derived and clarified. This takes us a step closer to understanding how BM can explain the optimized (or even the phase space) GHZ test, by allowing an in principle simulation.

2.5 Roy Singh Theory

Roy Singh (RS) proposed [RS95] a causal completion of QM, that treated position and momentum symmetrically. In their theory, the joint probability distribution was such that when the momentum is integrated out, the result agrees with quantum mechanical predictions for position *and* when positions are integrated out, they agree with the quantum mechanical momentum distribution. This was rather interesting for, BM fails to do the latter, and requires more analysis to resolve (as was discussed in the previous section). This joint probability distribution, given by RS, could indeed be thought of as describing the phase space of real particles, for it was positive everywhere, unlike the Wigner distribution.

The cost, however, was that evaluation of arbitrary functions of q, p was not as simple as integrating it over the joint distribution. While a promising framework and interesting in its own right, in the light of the optimized GHZ test, it wasn't particularly helpful. It was not pursued beyond a preliminary reading stage.

2.6 Remarks

In summary then, we have looked at a version of the GHZ test, the phase space extension. This effectively says that $\hat{q}, \hat{p}$ can't have pre-defined values. Now, even though BM has pre-defined values for q, p in principle, upon measurement, we learnt that the value of p can change. In fact, it may very well depend on the initial position of the measuring particle. To be able to test this quantitatively, we had to (a) optimize the phase space GHZ test, (b) learn more about measurements and (c) write an appropriate BM simulator. Progress was made on each front and the results discussed. However, the crucial point is that even in BM, the measurements correspond to operators. It entails therefore that measuring $ABC \neq D$ but in fact[1] $ABC = -D$, even from the point of view of BM, a deterministic theory. This hinges essentially on whether we can commute the operators that were used to construct A, B, and C to start with, which even in BM we can't. Stated another way, we learn that $YXY \neq Y^2X = X$, but $YXY = -Y^2X = -X$, even in BM, where these operators have pre-defined values (given all initial conditions). This is simply because X and Y are operators and they anti-commute. So even though numerically we haven't quite proven that BM will be consistent, qualitative cogent arguments already suggest that BM will in fact turn out to be consistent with QM. What will remain, will be a matter of detail.

[1] where A, B, C, D are as defined for the spin GHZ, and the argument essentially holds even for the phase-space (optimized) GHZ

Chapter 3

Contextuality and Bohmian Mechanics

3.1 Rationale

We saw in the last chapter that BM is able to explain the GHZ test. The paradox arises if we try to multiply values assigned to operators that don't commute, to obtain the value assigned to a product of such operators. In BM, since the operator must be provided to obtain its value, no contradiction arises even though the results are deterministic (given all initial conditions). Thus, we were only able to rule out the theories that treated operators like numbers and we find that BM is not one of them. However, as we have seen in the Peres Mermin (PM) test, the operators whose values are multiplied do in fact commute, implying that the PM test is exonerated from that objection. And we also know that BM, at least on the face of it, is non-contextual, viz. the value obtained by the measurement of an operator depends only on the state (+ hidden variables) and the operator, granted we fix our measurement scheme. It is therefore not clear how BM is contextual, which is a notion we're forced to accept from the PM test. Further, since BM is claimed to reproduce all results of QM, does it entail that a non-contextual theory can explain the PM test?

We also found in the previous chapter, that in BM, there's no fundamental difference that arises between the phase space variables and spins. As we saw, the value of momentum observed depends on the systematics of the measurement process, just as the outcome of a spin measurement using an SG setup (as was discussed in the first chapter). Therefore in what follows, attempts will be made at tackling the problem from whichever method (between phase space and spins) appears more accessible.

3.2 Intensifying Contextuality

We have already seen that GHZ test is a test of determinism, of whether predefined values can explain QM, while the PM test is that of contextuality, which says that predefined non-contextual values, a more subtle remark, can't explain QM. We also learnt how one can extend the GHZ test to continuous variables. In this section, we will make both these schemes effectively equally powerful; make GHZ into a test of contextuality and extend the PM test to continuous variables.

3.2.1 GHZ escalated to Contextuality

Recall from the first chapter, $\hat{A} \equiv \sigma_x \otimes \sigma_y \otimes \sigma_y$, $\hat{B} \equiv \hat{\sigma}_y \otimes \hat{\sigma}_x \otimes \hat{\sigma}_y$, $\hat{C} \equiv \hat{\sigma}_y \otimes \hat{\sigma}_y \otimes \hat{\sigma}_x$ and $\hat{D} = \hat{\sigma}_x \otimes \hat{\sigma}_x \otimes \hat{\sigma}_x$, and $\hat{A}\hat{B}\hat{C} = -\hat{D}$. Consider now, in addition, the following operators,

$$\hat{H}_{ij} \doteq \begin{bmatrix} \hat{\sigma}_x \otimes \hat{\mathbb{I}} \otimes \hat{\mathbb{I}}^{(a)} & \hat{\mathbb{I}} \otimes \hat{\sigma}_y \otimes \hat{\mathbb{I}}^{(2)} & \hat{\mathbb{I}} \otimes \hat{\mathbb{I}} \otimes \hat{\sigma}_y^{(3)} \\ \hat{\sigma}_y \otimes \hat{\mathbb{I}} \otimes \hat{\mathbb{I}}^{(1)} & \hat{\mathbb{I}} \otimes \hat{\sigma}_x \otimes \hat{\mathbb{I}}^{(b)} & \hat{\mathbb{I}} \otimes \hat{\mathbb{I}} \otimes \hat{\sigma}_y^{(3)} \\ \hat{\sigma}_y \otimes \hat{\mathbb{I}} \otimes \hat{\mathbb{I}}^{(1)} & \hat{\mathbb{I}} \otimes \hat{\sigma}_y \otimes \hat{\mathbb{I}}^{(2)} & \hat{\mathbb{I}} \otimes \hat{\mathbb{I}} \otimes \hat{\sigma}_x^{(c)} \\ \hat{\sigma}_x \otimes \hat{\mathbb{I}} \otimes \hat{\mathbb{I}}^{(a)} & \hat{\mathbb{I}} \otimes \hat{\sigma}_x \otimes \hat{\mathbb{I}}^{(b)} & \hat{\mathbb{I}} \otimes \hat{\mathbb{I}} \otimes \hat{\sigma}_x^{(c)} \end{bmatrix}$$

and note that (a) the product of these operators along each row yields $\hat{A}$, $\hat{B}$, $\hat{C}$ and $\hat{D}$ respectively, (b) operators along any row, commute and (c) the superscript labels identify operators that are repeated.

We will now try to assign values to $\hat{H}_{ij}$ and only multiply values assigned to commuting observables to obtain the value of $\hat{A}, \hat{B}, \hat{C}$ and $\hat{D}$. We know (see Section 1.5) that according to QM, for the GHZ state, $|\chi_G\rangle$, $\hat{A}$, $\hat{B}$ and $\hat{C}$ must be assigned the value $+1$, while $\hat{D}$ must be assigned -1. We demand that our assignment corresponds to this state. Let us start with assigning values to the last row. To obtain a -1 corresponding to D, we must have either a $1, 1, -1$ (or permutations) or $(-1, -1, -1)$. Let us assume that the former is true. At this stage then, we would have

$$H_{ij} \doteq \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \\ 1 & 1 & -1 \end{bmatrix}.$$

Now to obtain a $+1$ in the first row (for A), we must have $(1, \pm 1, \pm 1)$. Similarly we get, for the second row, $(\pm 1, 1, \pm 1)$. The assignment then becomes

$$H_{ij} \doteq \begin{bmatrix} 1 & \pm 1 & \pm 1 \\ \pm 1 & 1 & \pm 1 \\ \pm 1 & \pm 1 & -1 \\ 1 & 1 & -1 \end{bmatrix}.$$

However, we have no freedom left and are forced to assign -1 to the third row, while we were required to have it equal $+1$. A little reflection reveals that the $(-1, -1, -1)$ case for the last row, will not resolve the issue. Thus we conclude that the assignment must be contextual (atleast the one corresponding to $|\chi_G\rangle$). In this scenario, the non-commuting observables argument, deduced in the previous chapter fails. Here, values of only commuting observables were multiplied, even though effectively it is still the same GHZ test.

3.2.2 Peres Mermin escalated to Continuous Variables

The Peres Mermin situation can be, quite simply, extended to continuous variables, which may be of practical interest. Performing SG type setup in the simulation requires implementation of spins and appropriate magnetic field effects, and that can be surpassed with this construction. To this end, the following extension was worked out (but this result was already known [ABS+15]). For any unitary operators $\hat{X}$ and $\hat{Y}$, s.t. $\{\hat{X},\hat{Y}\}=0$ and so is $\{\hat{X},\hat{Y}^\dagger\}=0$, if we define $\hat{Z}=i\hat{Y}\hat{X}$, then

$$\begin{array}{ccc} \hat{X}\otimes\hat{\mathbb{I}} & \hat{\mathbb{I}}\otimes\hat{X} & \hat{X}^\dagger\otimes\hat{X}^\dagger \\ \hat{\mathbb{I}}\otimes\hat{Y} & \hat{Y}\otimes\hat{\mathbb{I}} & \hat{Y}^\dagger\otimes\hat{Y}^\dagger \\ \hat{X}^\dagger\otimes\hat{Y}^\dagger & \hat{Y}^\dagger\otimes\hat{X}^\dagger & \hat{Z}\otimes\hat{Z} \end{array}$$

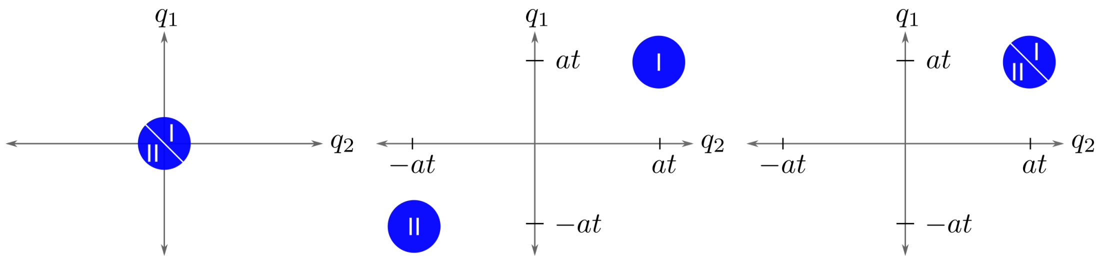
would yield the PM situation. To check this, note that the product along any row is $\hat{\mathbb{I}}$ and it is also so for each column, except for the third, which is $-\hat{\mathbb{I}}$; precisely the same as the PM situation. The difference however, will be that the corresponding hidden variables will have to be unimodular complex (viz. $XX^*=1$) and the values of the operators must be deduced from their hermitian counterparts. One such choice of X and Y was pointed out in the previous chapter; $\hat{X}\equiv e^{i\sqrt{\pi}\hat{q}/\hbar L}$ and $\hat{Y}\equiv e^{i\sqrt{\pi}\hat{p}L/\hbar}$. Note that in this case, optimization is not required, for this test is state independent (should work with any choice of states).

3.3 Measurements in BM (II)

Measurements have already been discussed at length in the previous chapters, however, we are now particularly interested in measuring spins, especially when there is entanglement. We will see how a measurement made using the Stern-Gerlach like apparatus can yield results very different from those obtained by the Hamiltonian approach. Further, we will see how the former can get difficult to evaluate, quite quickly.

3.3.1 Stern Gerlach based measurements

Since we have already discussed how to analyse a Stern-Gerlach based measurement for a single particle, let us try to explore how to analyse this for $|\chi\rangle=|{+}{+}\rangle+|{-}{-}\rangle/\sqrt{2}$, where for instance $|{+}{+}\rangle=|+\rangle_A\otimes|+\rangle_B$ (A and B label the particle), and $\hat{\sigma}_x\otimes\hat{\sigma}_x$ is the observable of interest. Borrowing the notation and the analysis from Section 1.4, we have $\sqrt{2}|\Psi_S\rangle=|\psi,\psi\rangle\otimes[|{+}{+}\rangle+|{-}{-}\rangle]$ initially and after the interaction, $\sqrt{2}|\Psi_S(t)\rangle=|\psi_{at},\psi_{at}\rangle\otimes|{+}{+}\rangle+$



(a) Initial State (b) For $\sqrt{2}|\chi\rangle = |00\rangle + |11\rangle$ (c) For $|\chi\rangle = |{++}\rangle$

Figure 3.1: Indicative contour plots for $|\langle q_1, q_2|\Psi_S\rangle|^2$, illustrating spin measurement of 2 particles, using the Stern Gerlach setup.

$|\psi_{-at}, \psi_{-at}\rangle \otimes |{--}\rangle$, where $|\psi_{at}, \psi_{at}\rangle = |\psi_{at}\rangle_A \otimes |\psi_{at}\rangle_B$ for example. Now, we must predict the outcome given the initial positions of the particles. We then plot $P(q_1, q_2) = \langle \Psi_S|q_1, q_2\rangle \langle q_1, q_2|\Psi_S\rangle$, where q_1 and q_2 represent the z coordinate of the particles, and effectively we are summing over the spin degree of freedom, asking for the probability of finding the particles near q_1 and q_2. Initially, $P = |\langle q_1, q_2|\psi, \psi\rangle|^2$ which would yield circles in a contour plot (showing say 70% probability enclosed within), see Figure 3.1a. After the interaction, $2P(q_1, q_2) = |\langle q_1, q_2|\psi_{at}, \psi_{at}\rangle|^2 + |\langle q_1, q_2|\psi_{-at}, \psi_{-at}\rangle|^2$, which would yield two circles in the contour plot, one centred at (at, at) and the other centred at $(-at, -at)$, see Figure 3.1b. From the symmetry of the problem and from the fact that velocities are single valued, we can deduce that if the particle positions were represented by a point inside area I, then the result would be a spin up, viz. $|+\rangle$ for both, while for the other case, the result would be spin down for both. Note that there's no initial condition for which the results are anti-correlated, consistent with $|\chi\rangle$. Although it is obvious, it is instructive to see how this would work for $|\chi\rangle = |{++}\rangle$ for instance. In this case also, the initial plot for P is identical to that shown in Figure 3.1a. However, since after the interaction, $|\Psi_S(t)\rangle = |\psi_{at}, \psi_{at}\rangle \otimes |{++}\rangle$, we see that $P = |\langle q_1, q_2|\psi_{at}, \psi_{at}\rangle|^2$, which is just a Gaussian centred at (at, at), as shown in Figure 3.1c. Now, regardless of the initial conditions of the particles, after the interaction, they will be carried to a Gaussian at (at, at) by the probability current (which is effectively their velocity). Thus, the result is always spin up, for both particles, consistent with QM.

It is straight forward to extend this analysis to the GHZ situation, with three particles. However, in that case, determining which area (in phase space, viz. the set of initial positions) corresponds to which outcome, becomes non-trivial, for certain operators. The difficulty arises from the increasing possible final states.

3.3.2 Hamiltonian Approach

We have already used the Hamiltonian approach in Section 2.4 and so extending it to spins will not be surprising. However, as we will see, it incredibly simplifies the measurement process.

3.3.2.1 Single Spin

Let the spin state of our particle, be $\sqrt{2}|\chi\rangle = |0\rangle + |1\rangle$ and let the spatial state of the measuring particle be $|\psi\rangle$. Neglecting the spatial wavefunction of the particle of interest, we can write the state of the entire system as $|\Psi_S\rangle = |\psi\rangle \otimes |\chi\rangle$. From Section 2.4, we know that the required Hamiltonian is $\hat{H} = a\hat{\sigma}_z \otimes \hat{p}$, given that we wish to measure $\hat{\sigma}_z$. Consequently, after the interaction, we get $\sqrt{2}|\Psi_S(t)\rangle = |\psi_{at}\rangle \otimes |0\rangle + |\psi_{-at}\rangle \otimes |1\rangle$. This has become mathematically identical to the SG based measurement discussed in Section 1.4. The results therefore, follow from our older discussions. Note that one can use this analysis as an alternative to show that spins can't be associated with a particle, effectively using the same arguments. However, to stress the difference, note that in the SG case, the position of the particle of interest itself determined whether the measurement would yield spin up or spin down. Here, the position of the particle of interest plays no role in the measurement scheme. In fact, the position of the measuring particle (which in some sense represents the apparatus) determines the outcome. Thus, even though in both cases, the result can be predicted, it is possible to have initial conditions such that the results of these two different measurement schemes don't match.

3.3.2.2 Entangled Spin

Let the spin state of the particles be $\sqrt{2}|\chi\rangle = |00\rangle + |11\rangle$ and let the position of the measuring particle be $|\psi\rangle$. Neglecting again, the spatial wavefunction of the two particles, we have, for the entire system, $|\Psi_S\rangle = |\psi\rangle \otimes |\chi\rangle$. If we wish to measure $\hat{\sigma}_z \otimes \hat{\sigma}_z$, (which must yield $+1$), we use $\hat{H} = a(\hat{\sigma}_z \otimes \hat{\sigma}_z) \otimes \hat{p}$. This yields $|\Psi_S(t)\rangle = |\psi_{at}\rangle \otimes |\chi\rangle$, which from the aforesaid arguments entails that for all initial positions of the measuring particle we would get $+1$. Since the result is $+1$, we obtain a result corresponding to correlated spins in the SG setup, with less effort.

3.3.2.3 GHZ Entangled Spin

Let the spin state now be $\sqrt{2}|\chi\rangle = |000\rangle - |111\rangle$, the case we couldn't analyse in a simple way earlier. Assume that we wish to measure $\hat{A} = \hat{\sigma}_x \otimes \hat{\sigma}_y \otimes \hat{\sigma}_y$. Since $\hat{A}|\chi\rangle = |\chi\rangle$, it follows that after the interaction we would have $|\Psi_S(t)\rangle = |\psi_{at}\rangle \otimes |\chi\rangle$, that'll yield $+1$ with certainty. Obtaining this conclusion from the SG formalism would've been much harder. Let us attempt something non-trivial; let us measure $\hat{\sigma}_x \otimes \hat{\mathbb{I}} \otimes \hat{\mathbb{I}}$. To proceed, we re-write the spin state as $\sqrt{2}|\chi\rangle = |+\rangle(|00\rangle - |11\rangle) + |-\rangle(|00\rangle + |11\rangle)$ and now observe that the state of the complete system after the interaction would be $\sqrt{2}|\Psi_S(t)\rangle = |\psi_{at}\rangle \otimes |+\rangle(|00\rangle - |11\rangle) + |\psi_{-at}\rangle \otimes |-\rangle(|00\rangle + |11\rangle)$. Now if the measuring particle was initially at $q > 0$, we would get a $+1$ value and the resultant state would be $|+\rangle(|00\rangle - |11\rangle)$ and similarly for $q < 0$, -1 and $|-\rangle(|00\rangle + |11\rangle)$.

3.4 Peres Mermin Revisited

With the tools for measurement sharpened, we are now in a position to explicitly assign values to the Peres Mermin situation and find out precisely how contextuality can be reconciled with BM. However, before proceeding with that, we first try to carefully list the restrictions made on the hidden variable theory. These are sufficient to arrive at a contradiction with QM.

3.4.1 Assumptions

According to QM, if one has a set of compatible operators, say $\hat{A},\hat{B},\hat{C}$ (some arbitrary operators), then one can construct simultaneous eigenkets $|a,b,c\rangle$. Now if the system is prepared in such a state, then the value obtained by measuring $\hat{A}\hat{B}\hat{C}$ is the same as that obtained by measuring $\hat{A},\hat{B}$ and $\hat{C}$ separately, in any order, and multiplying the result. We can arrive at a contradiction if we make the following three assumptions about the HV model. (1) Non-contextual assignment: The value assigned to any operator, depends only on the operator and the state of the system (including hidden variables). (2) Multiplicativity: Value assigned to the product of commuting operators must be the product of values assigned to the commuting operators themselves. (3) Non-Invasive: Measurement doesn't affect the remaining assignments.

It is already clear that relaxing requirements (2) and (3) might make the assignment consistent with QM, voiding the necessity of concluding contextuality.

3.4.2 BM explanation of Peres Mermin

Let us explicitly assign values to the PM situation to explore precisely which of the aforesaid assumptions goes wrong. For simplicity, let us assume that our state to start with, is $|\chi\rangle = |00\rangle$ and $q > 0$ for the measuring particle, initially. For convenience, we have re-written the relevant operators

$$\hat{A}_{ij} \doteq \begin{bmatrix} \hat{\mathbb{I}}\otimes\hat{\sigma}_x & \hat{\sigma}_x\otimes\hat{\mathbb{I}} & \hat{\sigma}_x\otimes\hat{\sigma}_x \\ \hat{\sigma}_y\otimes\hat{\mathbb{I}} & \hat{\mathbb{I}}\otimes\hat{\sigma}_y & \hat{\sigma}_y\otimes\hat{\sigma}_y \\ \hat{\sigma}_y\otimes\hat{\sigma}_x & \hat{\sigma}_x\otimes\hat{\sigma}_y & \hat{\sigma}_z\otimes\hat{\sigma}_z \end{bmatrix}.$$

Using results from Subsection 3.3.2.1, we know that operators for which $|\chi\rangle$ is an eigenvector, they will always yield the corresponding eigenvalue. In the present case, only $\hat{\sigma}_z\otimes\hat{\sigma}_z$ has $|\chi\rangle$ as an eigenket. Thus we assign it $+1$ (the eigenvalue). We will not present the details of calculations that yield the following predictions. They can however be easily motivated, by noting that each operator, can yield only a ±1 value, since $\hat{A}_{ij}^2 = \hat{\mathbb{I}}\otimes\hat{\mathbb{I}}$. By symmetry of the operators and the state, it follows that (one can check explicitly) each of these operators (for which $|\chi\rangle$ is not an eigenket), yield ± 1 with equal probability. Thus, the eigenket of these operators that corresponds to the $+1$ value, is the one that will correspond to $|\psi_{at}\rangle$. Since $q > 0$ by assumption, it follows that all these operators would yield $+1$, viz. the assignment will be

$$\begin{bmatrix} +1 & +1 & +1 \\ +1 & +1 & +1 \\ +1 & +1 & +1 \end{bmatrix}.$$

It is obvious that this assignment if we assume (2), will fail to be consistent with QM. However, since $\hat{R}_i = \mathbb{I}$ and $\hat{C}_j = \mathbb{I}(j \neq 3)$, $\hat{C}_3 = -\mathbb{I}$, $(\forall i, j)$ have $|\chi\rangle$ as an eigenket (in fact all possible states are eigenkets). According to BM, the value assigned will be $+1$ to all except C_3, which will be assigned -1. We learn therefore that in BM, (2) certainly doesn't hold. Also, since the wavefunction collapses after a measurement, we know that the assignment must change, in general, thus (3) also doesn't hold in BM. Finally, given an operator, BM can predict the value one would get upon measuring it, although one needs to specify the measurement process. Thus, we see, that (1) does in fact hold in BM, granted we restrict ourselves to a fixed measurement process.

3.5 Remarks

It was realised that the GHZ determinism test is not satisfactorily explained by the non-commuting observables being treated as numbers. An equivalence between the GHZ and the PM test was established, in terms of the conclusions. Consequently, tools required to find an explicit assignment for the PM situation were sharpened. From the assignment, it was found that a non-contextual theory doesn't contradict QM, viz. contextuality is not a necessary feature of QM. It was found with ambivalence, that contextuality has been questioned in the literature [LC09]. However, the arguments used and the construction of the counterexample vastly differs from those presented here. Our construction is considerably simpler.

Chapter 4

An Alternative to Contextuality

4.1 Rationale

In principle, we have achieved what we set out to; we were able to understand how BM explains PM, a test of contextuality. Having clarified various concepts through the heavy machinery of BM, here we attempt to further our understanding without using BM. We will start with refining the assumptions of the PM test. We will see how, when one of the assumptions is refined, one version holds for QM. The other is not even experimentally testable. Thereafter, we construct simple toy models, one of which is unambiguously non-contextual (unlike BM, where one must restrict the measurement process to make the same claim). This is used to demonstrate the distinction between the two versions of multiplicativity. We then generalize this toy model to produce statistics consistent with QM, for an arbitrary, but discrete Hilbert space. Finally, we generalize this to continuous variables (without spins) and obtain a consistent one-dimensional completion of QM. Its relation with other known completions (BM & RS) is also discussed. This model aims to facilitate easy value assignments in case of the phase space versions of determinism and contextuality tests. These are hard to compute from BM and RS.

4.2 Multiplicativity

Let us recall two assumptions from Section 3.4, that of non invasiveness and multiplicativity. Let $\hat{B}_1, \hat{B}_2, \ldots, \hat{B}_n$ be a set of commuting observables and also let $m_i(\hat{*})$ represent the value assigned to an operator. When m occurs multiple times in a given expression, then i encodes the sequence of measurements. If we assume non-invasiveness, then multiplicativity has a clear meaning;

Definition. In a Hilbert space $\mathscr{H}$, a map m_i from $\mathscr{H} \otimes \mathscr{H}^\dagger \to \mathbb{R}$, is *multiplicative* iff

$$m_1(f(\hat{B}_1, \hat{B}_2, \ldots \hat{B}_n)) = f(m_1(\hat{B}_1), m_1(\hat{B}_2), \ldots m_1(\hat{B}_n)). \tag{4.1}$$

Here we have generalized the notion from simply a product to any arbitrary function. We have used 1 as the subscript for each m since in this case, the sequence of a measurement is irrelevant. If one relaxes the no-disturbance assumption, then the following also becomes a possibility.

Definition. In a Hilbert space $\mathscr{H}$, a map m_i from $\mathscr{H}\otimes\mathscr{H}^\dagger \to \mathbb{R}$, is *sequentially-multiplicative* iff

$$m_1(f(\hat{B}_1,\hat{B}_2,\ldots,\hat{B}_n)) = f(m_{k_1}(\hat{B}_1),m_{k_2}(\hat{B}_2),\ldots m_{k_n}(\hat{B}_n)), \tag{4.2}$$

where $\mathbf{k} \equiv (k_1,k_2,\ldots k_n) \in \{(1,2,3,\ldots n),(2,1,3,\ldots n), +\text{ all permutations}\}$.

We take a moment to understand the meaning of these statements more carefully, in the context of QM. Consider the state $|\chi\rangle = |00\rangle$, $\hat{B}_1 \equiv \hat{\sigma}_x \otimes \hat{\sigma}_y$ and $\hat{B}_2 \equiv \hat{\sigma}_y \otimes \hat{\sigma}_x$ while $\hat{C} \equiv f(\hat{B}_1,\hat{B}_2) = \hat{B}_1\hat{B}_2 = \hat{\sigma}_z \otimes \hat{\sigma}_z$. Measuring $\hat{B}_1$ yields ± 1 with equal probabilities, and so does a measurement of $\hat{B}_2$. However, a measurement of $\hat{C}$ is guaranteed to yield $+1$. QM can't explicitly contradict Equation (4.1) since it only yields probabilities. Further, a measurement in QM leads to disturbance, unless of course we consider simultaneous eigenstates. Therefore, after making a measurement, say $m_1(\hat{B}_1)$, one can't obtain $m_1(\hat{B}_2)$. Even if we agree to start the measurement with the same state, we can't make the hidden variables identical. However, Equation (4.2) is certainly testable in QM, for one can first measure $\hat{B}_1$ to obtain $m_1(\hat{B}_1)$, then measure $\hat{B}_2$, to find $m_2(\hat{B}_2)$ and obtain $m_1(\hat{B}_1)m_2(\hat{B}_2)$. Starting from the state $|\chi\rangle$ again, one can measure $\hat{C}$ to get $m_1(\hat{C})$ which has a precise value in this case. One may again claim that experimentally, there maybe some hidden variables which can't be made identical and thus after measuring the Bs, it is impossible to obtain $m_1(\hat{C})$. This difficulty is circumvented in this case, by the fact that regardless of the value of the hidden variable, given $|\chi\rangle$ and $\hat{C}$, the measurement outcome is certain. Thus, taking the same state $|\chi\rangle$ is enough. One can check, from all the possibilities, if $m_1(\hat{B}_1)m_2(\hat{B}_2) = m_1(\hat{C})$. We tried looking for states and operators that would violate this condition, but failed. Infact, as we will prove momentarily, *QM weakly enforces sequentially multiplicative*. However, since restoring the hidden variables is not possible in general, *QM doesn't enforce multiplicativity*.

We worked out two proofs of weak sequential multiplicativity in QM. The first was a restricted, brute force proof. The second we showed holds in general, which we will discuss here.

Proposition. *Let the system be in a state, s.t. measurement of $\hat{C}$ yields repeatable results (same result each time). Then according to QM, sequential multiplicativity (see Equation (4.2)) holds, where $\hat{C} \equiv f(\hat{B}_1,\hat{B}_2,\ldots\hat{B}_n)$, and $\hat{B}_i$ are as defined.*

Proof. Assume without loss of generality that $\hat{B}_1,\hat{B}_2,\ldots\hat{B}_n$ are mutually compatible (commuting) and complete set of operators. If say for instance the set is not complete, then one can add the missing operators and label them as aforesaid. It follows that $\exists \left|\mathbf{b} = \left(b_1^{(l_1)}, b_2^{(l_2)}, \ldots b_n^{(l_n)}\right)\right\rangle$

s.t. $\hat{B}_i |\mathbf{b}\rangle = b_i^{(l_i)} |\mathbf{b}\rangle$, where l_i indexes the eigenvalues corresponding to $\hat{B}_i$ and that $\sum_{\mathbf{b}} |\mathbf{b}\rangle \langle \mathbf{b}| = \hat{\mathbb{I}}$. Let the state of the system be given by $|\psi\rangle$ and it must be s.t. $\hat{C}|\psi\rangle = c|\psi\rangle$, by assumption. For the statement to follow, one need only show that $|\psi\rangle$ must be made of only those $|\mathbf{b}\rangle$s, which satisfy $c = f(b_1^{(l_1)}, b_2^{(l_2)}, \dots b_n^{(l_n)})$. This is the crucial step. Proving this is so is trivial. We start with $\hat{C}|\psi\rangle = c|\psi\rangle$ and take its inner product with $\langle \mathbf{b}|$ to get

$$\begin{aligned} \langle \mathbf{b}|\hat{C}|\psi\rangle &= c\langle \mathbf{b}|\psi\rangle, \\ \langle \mathbf{b}| f(\hat{B}_1, \hat{B}_2, \dots \hat{B}_n)|\psi\rangle &= c\langle \mathbf{b}|\psi\rangle, \\ f(b_1^{(l_1)}, b_2^{(l_2)}, \dots b_n^{(l_n)})\langle \mathbf{b}|\psi\rangle &= c\langle \mathbf{b}|\psi\rangle. \end{aligned}$$

Also, we have $|\psi\rangle = \sum_{\mathbf{b}} \langle \mathbf{b}|\psi\rangle |\mathbf{b}\rangle$, from completeness. If we consider $|\mathbf{b}\rangle$s for which $\langle \mathbf{b}|\psi\rangle \neq 0$, then we can conclude that indeed $c = f(b_1^{(l_1)}, b_2^{(l_2)}, \dots b_n^{(l_n)})$. However, when $\langle \mathbf{b}|\psi\rangle = 0$, viz. $|\mathbf{b}\rangle$s that are orthogonal to $|\psi\rangle$, then nothing can be said. We can thus conclude that $|\psi\rangle$ is made only of those $|\mathbf{b}\rangle$s that satisfy the required relation. That completes the proof. □

Note that we can't enforce sequential multiplicativity in general, because of the hidden variable resetting objection that arises, which was discussed with the example. However, in the PM case, where $\hat{R}_i$ and $\hat{C}_j$ are just $\pm\hat{\mathbb{I}}$, it follows that all states are their eigenstates. Consequently, for these operators, sequential multiplicativity must always hold. With the two notions well defined, we now proceed with constructing two simple models, which don't satisfy the non-invasive assumption.

4.3 Simple Models

We aim to distinguish the notion of contextuality and multiplicativity by means of two simple models. These will not reproduce the statistics as predicted by QM, but serve as examples and are generalized later.

4.3.1 Contextual, Memory Model

The Memory Model presented here, is perhaps the simplest contextual model. It is also non-multiplicative and invasive, viz. it doesn't satisfy any of (1), (2) and (3), as listed in Section 3.4. The model is assumed to be sequentially multiplicative[1], and the assignments are made iteratively through the following algorithm. We assume that the system has a matrix that can store values and has a memory that can store the last 3 operators that were measured. Initially assume that the matrix has all entries equal to $+1$. The algorithm is that (i) upon measurement of an observable, yield the value as saved in the matrix, (ii) append

[1] infact according to QM, for row and column measurements, sequential multiplicativity is a requirement

the observable in the 3 element memory and (iii) update the matrix, once the context is known, to satisfy the PM conditions on the rows and columns.

Let us take a quick example to understand how things are working. Assume we start with measuring $\hat{A}_{33}$. The system will yield $m_1(\hat{A}_{33}) = 1$, in accordance with the values stored initially (see Equation (4.3)). The memory at this stage would read $\{*, *, \hat{A}_{33}\}$. Since the context is not yet known, the matrix is left unchanged. Say the next operator measured is $\hat{A}_{23}$. Then $m_2(\hat{A}_{23}) = 1$, and the memory would be updated to $\{*, \hat{A}_{33}, \hat{A}_{23}\}$. The context is now known, and we update the matrix to ensure that $m_1(\hat{C}) = m_1(A_{33})m_2(A_{23})m_3(A_{13}) = -1$. Since the first measurements yielded $+1$, we update the matrix so that $m_3(A_{13}) = -1$ to finally obtain the correct PM constraint. This has been summarized by the following equations.

$$m_1(\hat{A}_{ij}) = m_2(\hat{A}_{ij}) \doteq \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, m_3(\hat{A}_{ij}) \doteq \begin{bmatrix} 1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}. \tag{4.3}$$

The reader can convince her(him)self that the assignments are indeed consistent, regardless of which row/column is measured. There are two remarks which need to be made. First, note this model is not multiplicative since $m_1(\hat{A}_{33})m_1(\hat{A}_{23})m_1(\hat{A}_{13}) = 1 \neq m_1(\hat{C}) = -1$, by construction. Second, observe that the value assigned to the observables, depends explicitly on the context, thus the model is contextual.

4.3.2 Non-Contextual, Toy Model

We now discuss another simple model, which is non-contextual and still consistent with QM. It is also non-multiplicative and invasive, viz. assumption (1) holds, but (2) and (3) don't, as listed in Section 3.4. Reference to the PM square will be made, and it has been reproduced,

$$\hat{A}_{ij} \doteq \begin{bmatrix} \hat{\mathbb{I}} \otimes \hat{\sigma}_x & \hat{\sigma}_x \otimes \hat{\mathbb{I}} & \hat{\sigma}_x \otimes \hat{\sigma}_x \\ \hat{\sigma}_y \otimes \hat{\mathbb{I}} & \hat{\mathbb{I}} \otimes \hat{\sigma}_y & \hat{\sigma}_y \otimes \hat{\sigma}_y \\ \hat{\sigma}_y \otimes \hat{\sigma}_x & \hat{\sigma}_x \otimes \hat{\sigma}_y & \hat{\sigma}_z \otimes \hat{\sigma}_z \end{bmatrix},$$

for convenience. The assignments are made by a three step process.

1. Initial State: Choose an appropriate initial state $|\psi\rangle$ (say $|00\rangle$).
2. Hidden Variable (HV): Toss a coin and assign $c = +1$ for heads, else assign $c = -1$.
3. Predictions/Assignments: For an operator $\hat{p}' \in \{\hat{A}_{ij}, \hat{R}_i, \hat{C}_j\, (\forall i, j)\}$ check if $\exists$ a λ, s.t. $\hat{p}'\,|\psi\rangle = \lambda\,|\psi\rangle$. If $\exists$ a λ, then assign λ as the value. Else, assign c.

So far, the model has only predicted the outcomes of measurements. If however, a measurement is made on the system, then although we know the result from the predictions, we must update the state $|\psi\rangle$ of the system, depending on which observable is measured and arrive at new predictions, using the aforesaid steps. The following final step fills precisely

this gap.
4. Update: Say $\hat{p}$ was observed. If $\hat{p}$ is s.t. $\hat{p}\,|\psi\rangle = \lambda\,|\psi\rangle$, then leave the state unchanged. Else, find $|p_{\pm}\rangle$ (eigenkets of $\hat{p}$), s.t. $\hat{p}\,|p_{\pm}\rangle = \pm\,|p_{\pm}\rangle$ and update the state $|\psi\rangle \to |p_c\rangle$.

Let us explicitly apply the aforesaid algorithm, to the state $|\psi\rangle = |00\rangle$. Say we obtained tails, and thus $c = -1$. To arrive at the assignments, note that $|00\rangle$ is an eigenket of only $\hat{R}_i, \hat{C}_j$ and $\hat{A}_{33} = \hat{\sigma}_z \otimes \hat{\sigma}_z$. Thus, in the first iteration, all these should be assigned their respective eigenvalues. The remaining operators must be assigned c (see Equation (4.4)). Two remarks are in order. First, this model is *non*-multiplicative, for $m_1(\hat{C}_3) = -1 \neq m_1(\hat{A}_{13})m_1(\hat{A}_{23})m_1(\hat{A}_{33}) = 1$. Second, we must impose sequential multiplicativity as a consistency check of the model, which in particular entails that $m_1(\hat{C}_3) = m_1(\hat{A}_{33})m_2(\hat{A}_{23})m_3(\hat{A}_{13})$. To illustrate this, we must choose to measure $\hat{A}_{33}$. According to step 4 since $|00\rangle$ is an eigenstate of $\hat{A}_{33}$, the final state remains $|00\rangle$. For the next iteration, $i = 2$, say we again yield $c = -1$. Since $|\psi\rangle$ is also unchanged, the assignment remains invariant. For the final step, we choose to measure $\hat{p} = \hat{A}_{23}(= \hat{\sigma}_y \otimes \hat{\sigma}_y)$, to proceed with sequentially measuring $\hat{C}_3$. To simplify calculations, we note

$$|00\rangle = \frac{(|\tilde{+}\tilde{-}\rangle + |\tilde{-}\tilde{+}\rangle)/\sqrt{2} + (|\tilde{+}\tilde{+}\rangle + |\tilde{-}\tilde{-}\rangle)/\sqrt{2}}{\sqrt{2}},$$

where $|\tilde{\pm}\rangle = |0\rangle \pm i\,|1\rangle$ (eigenkets of $\hat{\sigma}_y$). Since $|00\rangle$ is manifestly not an eigenket of $\hat{p}$, we must find $|p_-\rangle$ since $c = -1$. It is immediate that $|p_-\rangle = (|\tilde{+}\tilde{-}\rangle + |\tilde{-}\tilde{+}\rangle)/\sqrt{2} = (|00\rangle + |11\rangle)/\sqrt{2}$, which becomes the final state.

$$
\begin{array}{c|ccc}
\text{Iteration} & i=1 & i=2 & i=3 \\
|\psi_{\text{init}}\rangle & |00\rangle & |00\rangle & \frac{|00\rangle+|11\rangle}{\sqrt{2}} \\
\text{HV/Toss} & c=-1 & c=-1 & c=+1 \\
\text{Predictions} & m_1(\hat{A}_{ij}) \doteq \begin{bmatrix} -1 & -1 & -1 \\ -1 & -1 & -1 \\ -1 & -1 & +1 \end{bmatrix} & m_2(\hat{A}_{ij}) \doteq \begin{bmatrix} -1 & -1 & -1 \\ -1 & -1 & -1 \\ -1 & -1 & +1 \end{bmatrix} & m_3(\hat{A}_{ij}) \doteq \begin{bmatrix} +1 & +1 & +1 \\ +1 & +1 & -1 \\ +1 & +1 & +1 \end{bmatrix} \\
\text{(Assignments)} & \begin{array}{c} m_1(\hat{R}_i), m_1(\hat{C}_j) = +1\,(j \neq 3) \\ m_1(\hat{C}_3) = -1 \end{array} & \begin{array}{c} m_2(\hat{R}_i), m_2(\hat{C}_j) = +1\,(j \neq 3) \\ m_2(\hat{C}_3) = -1 \end{array} & \begin{array}{c} m_3(\hat{R}_i), m_3(\hat{C}_j) = +1\,(j \neq 3) \\ m_3(\hat{C}_3) = -1 \end{array} \\
\begin{array}{c}\text{Operator} \\ \text{Measured}\end{array} & \hat{A}_{13} = \hat{\sigma}_z \otimes \hat{\sigma}_z; m_1(\hat{A}_{13}) = +1 & \hat{A}_{23} = \hat{\sigma}_y \otimes \hat{\sigma}_y; m_2(\hat{A}_{23}) = -1 & \hat{A}_{33} = \hat{\sigma}_x \otimes \hat{\sigma}_x; m_3(\hat{A}_{33}) = +1 \\
|\psi_{\text{final}}\rangle & |00\rangle & \frac{|00\rangle+|11\rangle}{\sqrt{2}} & \frac{|00\rangle+|11\rangle}{\sqrt{2}}
\end{array}
\tag{4.4}
$$

For the final iteration, $i = 3$, say we yield $c = 1$. So far, we have $m_1(\hat{A}_{33}) = 1$ and $m_2(\hat{A}_{23}) = -1$. We must obtain $m_3(\hat{A}_{13}) = 1$, independent of the value of c, to be consistent. Let's check that. According to step 3 since $\hat{\sigma}_x \otimes \hat{\sigma}_x (|00\rangle + |11\rangle)/\sqrt{2} = 1(|00\rangle + |11\rangle)/\sqrt{2}$, $m_3(\hat{A}_{13}) = 1$ indeed. As a remark, it maybe emphasised that the $m_2(\hat{A}_{33}) = m_3(\hat{A}_{33})$ and $m_2(\hat{A}_{23}) = m_3(\hat{A}_{23})$, which essentially expresses compatibility of these observables, viz. measurement of $\hat{A}_{13}$ doesn't affect the result one would obtain by measuring operators compatible to it (granted they have been measured once before).

While this model serves as a simple counter-example to the usual 'QM is contextual' conclusion one draws the PM situation, the model fails to yield the appropriate statistics. For instance, if we consider simply the state $\sqrt{2}|\psi\rangle = \cos\theta |{++}\rangle + \sin\theta |{--}\rangle$, then it follows that a measurement of $\hat{A}_{11} = \hat{\mathbb{I}} \otimes \hat{\sigma}_x$, would yield ± 1 with equal probability according to the toy model, whereas it (the probabilities) should depend on θ according to QM.[2]

4.4 Generic Models

In this section, we present arguably, the simplest HV theories, one of which is for spin like systems (discrete Hilbert space) while the other is for phase space (continuous Hilbert Space) for spin-less particles. These models are essentially non-contextual completions of QM, which facilitate easy computation of value assignment to operators.

4.4.1 Discretely C-ingle Theory

The state of the system is $|\chi\rangle$, defined on a discrete Hilbert space (spin like) and we wish to assign a value to an arbitrary operator $\hat{A} = \sum_a a |a\rangle \langle a|$, which has eigenvalues $\{a_{\min} = a_1 \leq a_2 \cdots \leq a_n = a_{\max}\}$. This theory has the following postulates:

1. Initial HV: Pick a $c \in [0,1]$, from a uniform random distribution.
2. Assignment/Prediction: The value assigned to $\hat{A}$ is given by finding the smallest a s.t.

$$c \leq \sum_{a'=a_{\min}}^{a} \left|\langle a'|\chi\rangle\right|^2.$$

A measurement of $\hat{A}$, would yield a.

3. Update: After measuring an operator, the state must be updated (collapsed) in accordance with the rules of QM.

To see how this works, we restrict ourselves to a single spin case. Say $|\chi\rangle = \cos\theta |0\rangle + \sin\theta |1\rangle$, and $\hat{A} = \hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1|$. Now, according to the postulates of this theory, $\hat{A}$ will be assigned $+1$, if $c \leq \cos^2\theta$, else $\hat{A}$ will be assigned -1. It follows then, from c being uniformly random in $[0,1]$, that the statistics agree with predictions of QM. The

[2] This was pointed out by Prof. Arvind.

reader can convince him(her)self that the said scheme works in general, specifically for the PM situation.

We can clearly see that the assignment is non-contextual since given an operator and a state (+ the hidden variable), the value is uniquely assigned. The assignment is non-multiplicative, because this scheme when applied to the PM situation, becomes effectively the same as the toy model (barring the statistics). We have already seen explicitly that the toy-model non-multiplicative. The theory is, of course, invasive as the state is updated after each measurement.

4.4.2 Continuously C-ingle Theory | Preliminary

The state of the system is $|\psi\rangle$, defined for a single spin-less particle, and we wish to assign a value to an arbitrary operator

$$\hat{A} = \int_{a_{\min}}^{a_{\max}} daa \left|a\right\rangle \left\langle a\right|.$$

This theory has the following postulates:
1. Initial HV: Pick a $c \in [0,1]$, from a uniform random distribution.
2. Assignment/Prediction: The value assigned to $\hat{A}$ is given by an a that satisfies

$$c = \int_{a_{\min}}^{a} \left|\psi(a')\right|^2 da',$$

where $\psi(a') = \langle a'|\psi\rangle$. A measurement of $\hat{A}$, would yield a.
3. Update: After measuring an operator, the state must be updated (collapsed) in accordance with the rules of QM.

The continuous variable version has some exclusive interesting features. First, note that for $\hat{A} = \hat{q}$ (the position), one can predict the trajectory of a particle. This is quite intuitive to observe graphically. Say c had a value as shown in the graph (see Figure 4.1) and the initial state is given by a Gaussian. Now the cumulative of this can be quickly constructed, and where the c line intersects the graph, that will yield the position of the particle. At some later time if the Gaussian shifts (assume it had some momentum), then for the same value of c, the particle's location would've moved with the Gaussian as expected. In fact, this is a general feature and can be done for all observables, including p. The theory is explicitly non-contextual since values are uniquely assigned to operators, given ψ and c. However, one needs more analysis to extend this to multiple particles. Once that is accomplished, one must show that measuring the observables using the Hamiltonian approach, would yield results consistent with those obtained from the postulates of the theory. To show then that the theory is non-contextual, one would be required to show that all concievable measurement schemes would produce the same result, else, like BM, this

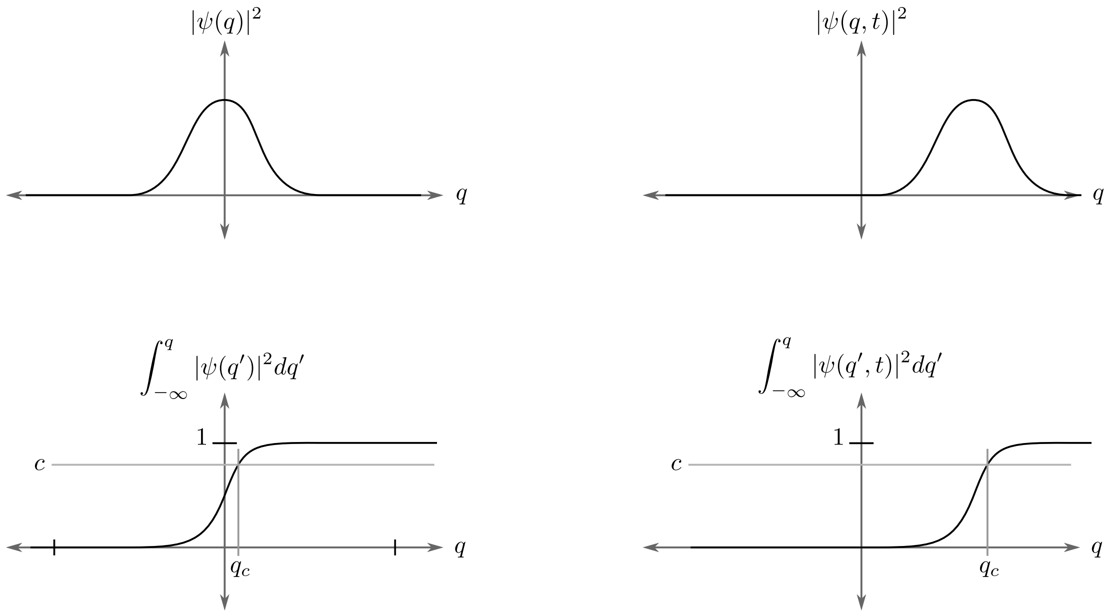


Figure 4.1: Illustration of the underlying principle of the continuously c-ingle model

theory wouldn't be able to predict the values of operators with only the state and hidden variable information. Once extended appropriately, this theory would effectively overcome all the challenges we had for testing the continuous variable extensions of the GHZ and contextuality tests. Predictions of observables will be straight forward. To obtain values from BM, one had to do a detailed analysis, for RS, evaluating values of observables other than q and p (even $q+p$ is hard) was hard.

We had this hunch however, that the trajectory so obtained, must be identical to Bohmian trajectories. This infact turns out to be so. Let us take a moment to prove this, for using the same method, one can evalute a trajectory for the momentum also. This would be distinct from the momentum in BM. In this case, a measurement of $\hat{p}$ yields p (the assigned value), unlike in BM.

Proposition. *$\dot{q} = \nabla S/m$ in a continuously c-ingle theory, for a single particle, with one degree of freedom.*

Proof. Let f quantify some property of a particle. To point to a particle, we can either use the variables c,t or x,t since we know how x and c are related. Thus, one can write $f(c,t)$ or $f(x,t)$.[3] Now we have

$$\left[\frac{\partial f}{\partial t}\right]_c = \left[\frac{\partial f}{\partial t}\right]_t \cdot \left[\frac{\partial q}{\partial t}\right]_c + \left[\frac{\partial f}{\partial t}\right]_q,$$

where we used $f(x,t)$ on the RHS. Note also that $\dot{q}$ refers to the velocity of a given particle, thus it must equal $[\partial q/\partial t]_c$. Now for $f = \int_{-\infty}^{q} |\psi(q')|^2 dq' = c$, the LHS disappears.

[3] If you think that the two functions should be different, then the notation is confusing you. $f(x,t) = f(t,x)$ should help resolve. The position of the arguments is not important, this is not like a computer function. $f(x,t)$ is the statement that f is a function of x,t. That's it.

Consequently, we have

$$\left[\frac{\partial q}{\partial t}\right]_c = -\left[\frac{\partial f}{\partial t}\right]_q \Big/ \left[\frac{\partial f}{\partial q}\right]_t,$$

which is in a form which can be evaluated directly from the relation given. $[\partial f/\partial q]_t = |\psi(q,t)|^2 = R^2$, if $\psi = Re^{iS/\hbar}$. It is easy to show that the probability current is given by $\nabla S/m$. Using $[\partial\,|\psi(q,t)|\,/\partial t]_q = -\nabla.(R^2\nabla S/m)$, which is effectively the probability conservation statement, derived from Schrodinger's equation, written in polar form, it follows that $-[\partial f/\partial t]_q = R^2\nabla S$. Thus we have $\dot{q} = \nabla S$ as claimed. □

An equation similarly for $\dot{p}$ can be obtained and an appropriate dynamics can perhaps then be constructed. It may be mentioned as a remark that, quite independent of its motivation, this scheme can be used to compute Bohmian trajectories. It is much more efficient, as is apparent from a comparison of the resources required between computing an integral and the steps listed in Section 1.4.

4.5 The Verdict: Contextuality vs. Non-Multiplicativity

We have already constructed an explicit non-contextual model, which is consistent with QM. This model we knew had to be non-multiplicative. We will see how non-multiplicativity gives rise to what one might confuse to mean contextuality.

The approach is to take some compatible observables and to construct a 'super-operator', a measurement of which can yield the values of all of these compatible observables in a single shot. We would see then, that the in-principle measurement outcome of observing these compatible operators, would not be consistent. Now this one might treat as contextuality, but according to the definition in Section 3.4, we note that this is non-multiplicativity, as per Section 4.2.

Let us construct an explicit situation and make more precise statements. Borrowing the notation from Section 4.2, imagine

$$\hat{B}_1 = \hat{\sigma}_z \otimes \hat{\mathbb{I}} = |00\rangle\langle 00| + |01\rangle\langle 01| - [|10\rangle\langle 10| + |11\rangle\langle 11|],$$

$$\hat{B}_2 = \hat{\mathbb{I}} \otimes \hat{\sigma}_z = |10\rangle\langle 10| + |11\rangle\langle 11| - [|00\rangle\langle 00| + |01\rangle\langle 01|],$$

while we define

$$\hat{C} = f(\{\hat{B}_i\}) = 0.\,|00\rangle\langle 00| + 1.\,|01\rangle\langle 01| + 2.\,|10\rangle\langle 10| + 3.\,|11\rangle\langle 11|.$$

$\hat{C}$ maybe viewed as a function of $\hat{B}_1$, $\hat{B}_2$ and other operators $\hat{B}_i$ which are constructed to obtain a maximally commuting set. A measurement of $\hat{C}$, will collapse the state into one of the states which are simultaneous eignkets of B_1 and B_2. Consequently, from the observed value of $\hat{C}$, one can deduce the values of $\hat{B}_1$ and $\hat{B}_2$. Now consider $\sqrt{2}|\chi\rangle = |10\rangle + |01\rangle$, for which $m_1(\hat{B}_1) = 1$, and $m_1(\hat{B}_2) = 1$, using the discretely c-ingle theory (Subsection 4.4.1), with $c < 0.5$. However, $m_1(\hat{C}) = 1$, from which one can deduce that B_1 was $+1$, while B_2 was -1. This property itself, one may be tempted call contextuality, viz. the value of B_1 depends on whether it is measured alone or with the remaining $\{B_i\}$. However, it must be noted that B_1 has a well defined value, and so does $\hat{C}$. Thus by our accepted definition, there's no contextuality. It is just that $m_1(\hat{C}) \neq f(m_1(\hat{B}_1), m_1(\hat{B}_2), \dots)$, viz. the theory is non-multiplicative. Note that after measuring $\hat{C}$ however, $m_2(\hat{B}_1) = +1$ and $m_2(\hat{B}_2) = -1$ (for any value of c) consistent with those deduced by measuring $\hat{C}$.

4.6 Denouement

We have already learnt that the proof of 'contextuality', in fact requires three assumptions, (1) multiplicativity, (2) non-contextuality and (3) non-invasiveness. Here we were able to construct an explicit non-contextual theory (for spins) which is non-multiplactive, but invasive and completely consistent with QM. Succinctly stated, it satisfies (2) but neither (3) nor (1), serving as a counter-example to the claim that non-contextual hidden variable theories can't be consistent with QM. We also showed how the theory might be misconstrued to be contextual and provided a clarification. This is of interest because, in BM, contextuality can arise from two sources, one is the PM situation and second is the measurement process. These two usually get misconstrued and have engendered confusion about the said notion.

Chapter 5

Epilogue

5.1 Implications

In this section, non-contextuality (see Section 3.4) will be assumed and notation will be borrowed from Section 4.2. We will use our understanding from multiplicativity, to investigate its relationship between entanglement, locality, and superposition.

5.1.1 Superposition

It is known that for simultaneous eigenstates of $\hat{B}_i$, multiplicativity must hold. Consequently, any violation of multiplicativity must arise from states that are superpositions (of the simultaneous eigenkets). Note however, that entanglement is not necessary to show a violation, since the PM test is a state independent test, where a separable state can be used to arrive at a contradiction.

5.1.2 Non Locality and Entanglement

It is known from Section 1.3 that $\langle \hat{B} \rangle \leq 2$, where $\hat{B}$ is the Bell operator as defined there. If we assume (1), (2) and (3), as given in Section 3.4, then also it can be proven that $\langle \hat{B} \rangle \leq 2$. To see this, consider $\hat{B}_1 = \hat{a}_1 \otimes \hat{\mathbb{I}}$ and $\hat{B}_2 = \hat{\mathbb{I}} \otimes \hat{b}_1$, so that $[\hat{B}_1, \hat{B}_2] = 0$ and $\hat{C} \equiv \hat{B}_1 \hat{B}_2$. From multiplicativity, it follows that $m_1(\hat{C}) = m_1(\hat{B}_1) m_1(\hat{B}_2)$. This entails that $m(\hat{a}_1 \otimes \hat{b}_1) = m(\hat{a}_1 \otimes \hat{\mathbb{I}}) m(\hat{\mathbb{I}} \otimes \hat{b}_1)$, where the subscript has been suppressed for brevity. Note that $m(\hat{*})$, will depend on the state $|\psi\rangle$ and the hidden variables. Therefore, averaging multiple measurements, corresponds to averaging over the hidden variables. This is expressed by $\langle m(\hat{a}_1 \otimes \hat{b}_1) \rangle = \langle m(\hat{a}_1 \otimes \hat{\mathbb{I}}) \rangle \langle m(\hat{\mathbb{I}} \otimes \hat{b}_1) \rangle$. One can repeat this argument for each term in $\langle \hat{B} \rangle$. Using the fact that $-1 \leq m(\hat{*}) \leq 1$, and that the extrema will occur only at the extreme values of m, one can plugin ± 1 for each $\langle m(\hat{*}) \rangle$ to obtain $\langle \hat{B} \rangle \leq 2$. We can therefore conclude that a violation of Bell's inequality, entails that atleast one of the three assumptions is wrong.

One can infact try to show how a consistent (with QM) non-multiplicative theory, must be non-local. Formally it is clear, since a violation of Bell's inequality implies non-locality. Consequently, any consistent completion of QM, will be non-local. More insight can be gained, although some care is needed. The notion of compatible observables is that commuting observables don't disturb each other and can be simultaneously known. While the statement is not precisely stated, we only need to note that $m_{k_1}(\hat{C}) = m_{k_2}(\hat{B}_1)m_{k_3}(\hat{B}_2)$, for $(k_1,k_2,k_3) \in \{(1,2,3),(2,1,3),\dots\}$. In words, this means that to measure $\hat{C}$, one can instead first measure $\hat{B}_1$ and then measure $\hat{B}_2$. A multiplication of the values obtained, can be taken to be the value a measurement of $\hat{C}$ yields. This can be verified by measuring $\hat{C}$ subsequently. The Bell scenario offers an interesting freedom, by restricting the form of $\hat{B}_i$. To evaluate $\langle \hat{B} \rangle$, one is required to evaluate $\langle \hat{B}_1\hat{B}_2 \rangle$. From the compatibility argument, we need to find the average value of $m_3(\hat{B}_1\hat{B}_2) = m_1(\hat{B}_1)m_2(\hat{B}_2)$, viz. $\langle m_3(\hat{a}_1 \otimes \hat{b}_1) \rangle = \langle m_1(\hat{a}_1 \otimes \hat{\mathbb{I}}) \rangle \langle m_2(\hat{\mathbb{I}} \otimes \hat{b}_1) \rangle$. So far, the statements were general. Now we assume that our theory is non-multiplicative (and non-contextual). A consistent theory (with QM), using these assumptions, can and must violate $\langle \hat{B} \rangle \leq 2$. However, if the particles are taken far away, then the only way the theory can be non-multiplicative ($m_1(\hat{B}_1) \neq m_2(\hat{B}_1)$ for example), is if the theory is non-local. Locality will entail that $m_1(\hat{B}_1) = m_2(\hat{B}_1)$ for instance, since the information about which observable was measured first, can't be propagated instantaneously. We see therefore that non-locality arises quite naturally in consistent non-multiplicative theories.

As a remark, it may be added that in the case of the Bell Test, entanglement is needed to show one of the three assumptions is wrong. This is so because it can be shown that entanglement is necessary to arrive at a violation of the inequality.

5.2 Summary of Results

Progress was made roughly in three categories, as listed.

- Bohmian Mechanics
  - Generalized the Hamiltonian based measurement scheme to continuous variables (see Subsection 2.4.1.1)
  - Analytic/graphical proof of consistency check using position measurements (see Subsection 2.4.1.2)
  - Analytic/graphical solution to measuring entangled spins using SG & using the Hamiltonian scheme (see Subsection 3.3.1, Subsection 3.3.2)
  - Alternative proof of spins can't be associated with particles, and must only be a property of the wavefunction (see Subsection 3.3.2)

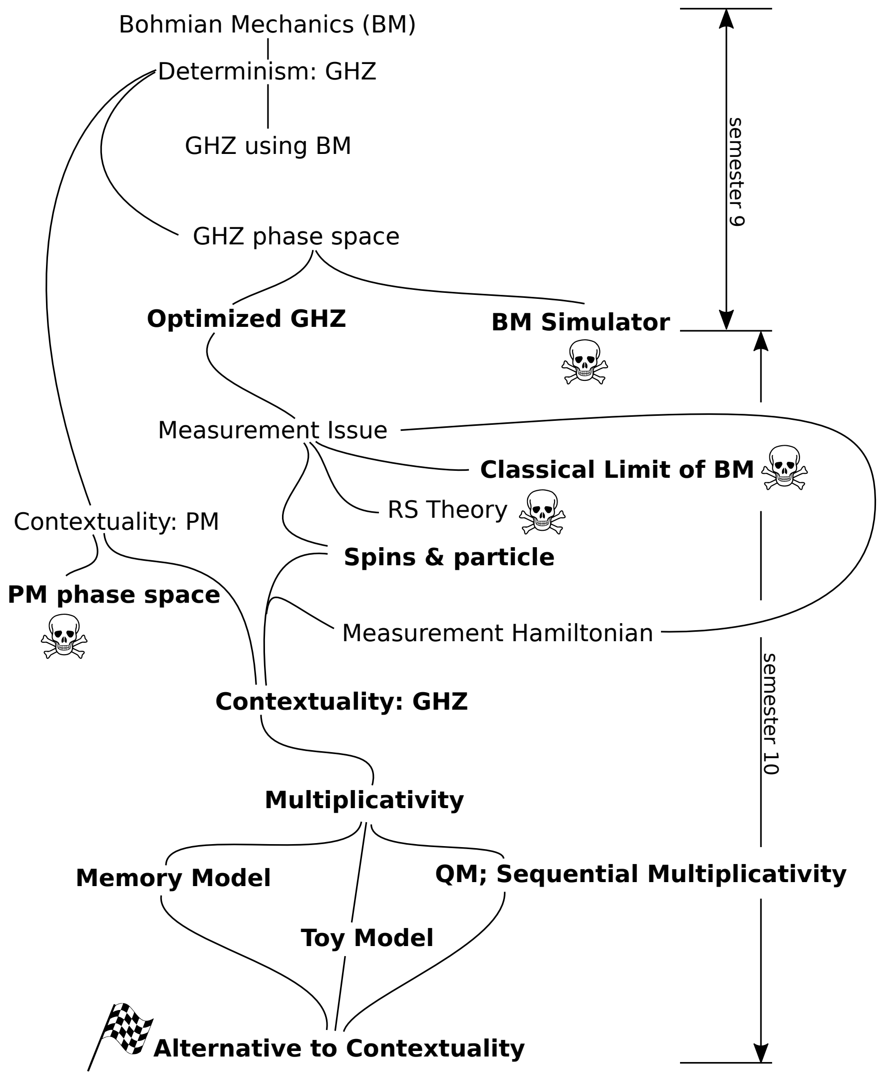


Figure 5.1: Overview of work done during the semesters. The bold faced titles represent new results.

  - BM simulator with many trajectories (one particle, one dimensional, arbitrary potential, see Section 2.3)

- Tests of Determinism and Contextuality

  - Optimized the phase space GHZ test (see Subsection 2.2.2.2)
  - GHZ $\rightarrow$ a test of contextuality (see Subsection 3.2.1)
  - PM extension to phase space (independently re-discovered, see Subsection 3.2.2)

- The Contextuality situation

  - BM was shown consistent with PM & restricted BM was argued to be non-contextual (see Subsection 3.4.2)
  - 'Multiplicativity' and 'Sequential Multiplicativity' identified, defined and proven where they hold (see Section 4.2)
  - Demonstrated 'non-multiplicativity' as an alternative to contextuality, by constructing a toy model (see Subsection 4.3.2)
  - Proposed the 'discretely c-ingle' HV theory to non-contextually explain spins (see Subsection 4.4.1)

5.3 Conclusion

We have shown, that atleast from the Peres Mermin's proof, it doesn't follow that contextuality is a necessary feature of QM. We have identified a new property, which we call non-multiplicativity. We have been able to construct a non-contextual hidden variable theory, that is completely consistent with QM of spins and it's predictions, we call a discretely c-ingle theory. This theory is non-multiplicative.

We also noted that upon restriction of measurement schemes, Bohmian Mechanics (BM) can also be viewed as a non-contextual hidden variable theory, which is non-multiplicative.

5.4 Digressions

As would've been evident so far, the developments made to address the main problem itself have not always been in the correct direction. In addition, certain small digressions were made, some of which have been listed for completeness.

5.4.1 Cryptography using contextuality

Interesting collaborative progress was made in developing certain cryptography protocols using contextuality, with Jaskaran and Kishor, who primarily constructed the schemes. A well-known idea is to use entanglement to facilitate secure sharing of keys, where the security assurance comes from the monogamy of Bell's inequality violations. An analogue of this idea was used, where the contextuality inequalities are used in place of Bell's and it was found that the said method is encouragingly secure and less resource hungry.

5.4.2 Attempt at superluminal communication with BM

Imagine there are two particles, one with person A, and the other with person B. Now both measure the position of their particles. Thus the positions are precisely known. Next, they allow their particles to evolve under a Hamiltonian (interaction) such that they become entangled. Suppose at time t, the particles are entangled. Now from the de-Broglie theory, both can predict the locations of their particles at t. Now comes the interesting part. The protocol they follow is as follows. Say A uses this setup, only to receive signals. If B wants to send a signal to A, all that he needs to do is to disturb his particle at t. This would cause some change in, either the wavefunction or the position, or both, of the particle, compared to if B had not caused any disturbance. Now, A measures her particle's position at $t+\varepsilon$ and gets the value q_A. She knows what position her particle should've been at, if B didn't do anything, call this position $q_A^{(0)}$. If now $q_A \neq q_A^{(0)}$, then she knows B sent a signal. If $q_A = q_A^{(0)}$, then she knows nothing was sent. Since the equations are non-local, this interaction is instantaneous, and in principle faster than the speed of light.
Ofcourse, one can fill in the details, which is what I almost started doing, but finding the fault in the argument is what was pivotal. It turns out, the fault was rather straight forward, although a little subtle. The idea is that regardless of how precise the position measurement is, its uncertainty will spread with the wavefunction, thereby rendering any prediction useless. Thus, in this light, chaos restores locality. This is actually not too hard to see. Imagine you have an uncertainty δq, when you measured the position and got the value q. Now we can imagine a gaussian associated with this, as the wavefunction, after the collapse. Since the de-Broglie Bohm theory ensures that the probability distribution $|\psi|^2$ is preserved by the dynamics of the particles, as ψ evolves, δq will increase (in the case of free evolution), effectively destroying 'position information'. The idea can only be harnessed if one can somehow decouple the uncertainty in q from the wavefunction.

5.4.3 Identical Particles, an alternate approach

One difficulty faced when we construct a statistical description of classical particles, is the Gibbs Paradox. At its heart, is the idea that one can always distinguish particles, on the basis of their paths. In QM, identical particles are handled quite elegantly, by (anti-)symmetrization of the wavefunction. In BM however, the trajectories are again well known and one might imagine that this signals failure of BM. It so turns out, that upon appropriately constructing the trajectory space, invariant under permutations of particles, one is able to stay consistent with QM and infact, able to gain further insights.

We realized however, that since QM describes reality, only through a combination of operators and the state, and that one can take the view that it is the observer that is incapable of distinguishing which particle is being looked at, therefore one can imagine that (anti-)symmetrizing operators should yield effectively the same results as (anti-)symmetrizing the wavefunctions.

As an illustration, consider the state $|\psi\rangle = |01\rangle$. If this state represented bosons, then we'd have to write according to the usual methods of QM, $\sqrt{2}|\psi_{\mathrm{I}}\rangle = |01\rangle + |10\rangle$. Now if we measure say $\hat{\sigma}_z \otimes \hat{\mathbb{I}}$, on $|\psi\rangle$, we'd obtain $+1$, while the same measurement on $|\psi_{\mathrm{I}}\rangle$ would yield 0 (on an average, in this case). However, if we instead symmetrize the operator as $(\sigma_z \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_z)/2$, then even if we measure $|\psi\rangle$, then on average. We'd get 0 upon measuring $|\psi_{\mathrm{I}}\rangle$ also, as is expected.

I was told by Prof. Mukunda that this has been discussed earlier by Messiah and Greenberg [MG64], in the context of particle physics. However when considered in view of the Bohmian formalism, it might yield an interesting alternative to the problem of identical particles.

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