Lecture Notes V: Quantum Fundamentals and Bose-Einstein Condensation

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1 Bell Inequalities

Physicists have had a complex relationship with the foundations of quantum mechanics. The study of the foundations of quantum mechanics[1] was long dismissed by senior physicists because, despite the conceptual difficulties, the theory worked so well. One of the greatest advances in our understanding of these concepts was advanced by John Bell in the 1960's as a long overdue response to the Einstein-Podolsky-Rosen (EPR) thought experiment of 1935. Let's try to understand the original EPR paradox and Bell's idea which helped to solidify our confidence that quantum mechanical state vectors are, in fact, complete descriptions of physical systems.

1.1 Entangled states

An n-particle system is in an *entangled state* if it's full state vector cannot be written as the direct product of n individual state vectors. Let's use a system of two distinguishable spin 1/2 particles as an example. The following state can be decomposed into two independent systems:

$$|\psi\rangle_{AB} = |\uparrow\uparrow\rangle = |\uparrow\rangle_A \otimes |\uparrow\rangle_B \tag{1}$$

but

$$|\psi\rangle_{AB} = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \tag{2}$$

has no such decomposition.

Quick Question: The state vector in (2) is one of four Bell states for a system of two spin 1/2 particles. Can you guess what the other three might be?

Much work has been put into understanding these states, and there are general ways of determining whether a state is an entangled state or not. Sometimes it's not

[1] Questions about the nature of measurements, the interpretation of the theory, the completeness of the theory, etc.

obvious! In this class we will stick to states which are 'clearly' not separable so we don't have to worry about this complication.

1.2 Bohm's realization of the Einstein-Podolsky-Rosen paradox

In 1935, Einstein published a paper with Boris Podolsky and Nathan Rosen proposed a thought experiment which they believed showed that quantum mechanics was an incomplete description of reality. They did not question whether quantum mechanics was correct, which had been experimentally verified, but whether it was complete. First, they proposed the following criteria for what they meant by a complete description:

1. Every element of the physical reality must have a counter part in the physical theory.
2. If, without in any way disturbing a system, we can predict with certainty (i.e. with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity.

Next, they proposed an experiment for which they believed that the quantum mechanical description did not satisfy these criteria. This is referred to as the EPR paradox. The original EPR paradox used a state with entangled positions and momenta, but David Bohm's version is both simpler to understand and experimentally realizable. The EPRB experiment is performed as follows. The decay of a spin 0 particle will produce a pair of particles. Conservation laws and spin statistics require that these particles travel in opposite directions and are of the form (2), we will call this an EPRB state.

Allow the particles to separate to a distance l sufficiently far that the timescale τ of an SGz measure is shorter than the time required for information to travel at the speed of light between the two particles (i.e. $l \gg c\tau$)[2]. When particle A is subjected to measurement by an SGz device, the outcome of the measurement is equally likely to be up or down. Suppose it was measured to be up. Then the state has collapsed to

$$|\psi\rangle = |\uparrow\downarrow\rangle \tag{3}$$

If particle B is immediately measured with another SGz device, it will always be deflected down.

This is what Einstein referred to as 'spooky action at a distance.' Quantum theory predicts that the first measurement changes the state of the second particle, even though it is too far away for it to do so immediately. The EPR paper rejected the possibility that the measurement of A could influence the state of B. This experiment would then imply the existence of some underlying theory which predicts the outcome

[2]Special relativity requires that information cannot travel faster than the speed of light.

from the beginning. Quantum mechanics would merely be an approximation to the underlying theory.

What does it mean for there to be an underlying theory? In a more compact form, what we are saying is that the probability of measuring first A up and then B down does not separate:

$$P(\uparrow_A, \downarrow_B) \neq P(\uparrow_A)P(\downarrow_B) \tag{4}$$

Statistically speaking, the outcomes of A and B are correlated rather than independent. However, suppose that there was some other quantity λ[3] which we simply hadn't been considering[4]. In that case, we might be able to write

$$P(\uparrow_A, \downarrow_B; \lambda) = P(\uparrow_A; \lambda)P(\downarrow_B; \lambda) \tag{5}$$

You should read the notation $P(A; \lambda)$ as "the probability of the outcome A given the specific value of λ." EPR called λ a hidden variable. An underlying theory would make explicit the dependence on this hidden variable, and predict outcomes according to (5). If this variable remains hidden, we would observe outcomes averaged over this variable. Supposing that the original preparation of the system had produced various values of λ, each with probability $f(\lambda)$, then the observed probabilities would be:

$$P_{\text{observed}}(\uparrow_A, \downarrow_B) = \sum_\lambda f(\lambda)P(\uparrow_A; \lambda)P(\downarrow_B; \lambda) \tag{6}$$

1.3 The Bell inequalities

Bell showed in the 1960's that a hidden variable theory could be distinguished from quantum mechanics in certain types of EPR experiments. Suppose that instead of SGz experiments on A and B, we perform the SG experiment on A (B) at an angle α (β) with the z-axis. Notice that α and β are *local* properties of the SG detectors. Then the probabilities for various outcomes are given by

$$P(\uparrow_A, \uparrow_B; \alpha, \beta) = P(\downarrow_A, \downarrow_B; \alpha, \beta) = \frac{1}{2}\sin^2\frac{\alpha-\beta}{2} \tag{7}$$

$$P(\uparrow_A, \downarrow_B; \alpha, \beta) = P(\downarrow_A, \uparrow_B; \alpha, \beta) = \frac{1}{2}\cos^2\frac{\alpha-\beta}{2} \tag{8}$$

One useful quantification of the correlations is the average value for the product of the two SG measurements, $\langle S_\alpha S_\beta \rangle$. We will suppress the $\hbar/2$ factors to keep the notation cleaner. In terms of probabilities, this is:

$$E(\alpha, \beta) = P(\uparrow_A, \uparrow_B; \alpha, \beta) + P(\downarrow_A, \downarrow_B; \alpha, \beta) - P(\uparrow_A, \downarrow_B; \alpha, \beta) - P(\downarrow_A, \uparrow_B; \alpha, \beta) \tag{9}$$

The positive (negative) terms are those where the outcomes have the same (different) sign so that their product must be positive (negative). I believe the letter E is chosen

[3]Assume λ takes discrete values, this does not change any results but simplifies our math.

[4]See page 152 of the Bell article from the Day 4 article for an example in which this is possible.

for this quantity to stand for *expectation value*, a fancy term for the expected average in the limit of a large number of samples.

Let's consider the quantum mechanical prediction for the quantity $E(\alpha,\beta)$. From (7) and (8), we find that

$$E_{\text{quantum}}(\alpha,\beta)=\sin^2\frac{\alpha-\beta}{2}-\cos^2\frac{\alpha-\beta}{2}=-\cos(\alpha-\beta) \tag{10}$$

Now consider the prediction if we have a hidden variable λ such that the quantum mechanical predictions are really averages as in (6). Then

$$\begin{aligned}E_\lambda(\alpha,\beta)&=\sum_\lambda E(\alpha,\beta,\lambda)\\&=\sum_\lambda f(\lambda)\left[P_A(\uparrow;\alpha,\lambda)P_B(\uparrow;\beta,\lambda)+P_A(\downarrow;\alpha,\lambda)P_B(\downarrow;\beta,\lambda)\right.\\&\qquad\left.-P_A(\uparrow;\alpha,\lambda)P_B(\downarrow;\beta,\lambda)-P_A(\downarrow;\alpha,\lambda)P_B(\uparrow;\beta,\lambda)\right]\\&=\sum_\lambda f(\lambda)\left[P_A(\uparrow;\alpha,\lambda)-P_A(\downarrow;\alpha,\lambda)\right]\left[P_B(\uparrow;\beta,\lambda)-P_B(\downarrow;\beta,\lambda)\right]\end{aligned} \tag{11}$$

Now, the P functions are probabilities such that

$$0\le P_A\le 1,\qquad 0\le P_B\le 1 \tag{12}$$

Equivalently, if we define

$$\bar{A}(\alpha,\lambda)\equiv P_A(\uparrow;\alpha,\lambda)-P_A(\downarrow;\alpha,\lambda) \tag{13}$$
$$\bar{B}(\alpha,\lambda)\equiv P_B(\uparrow;\beta,\lambda)-P_A(\downarrow;\beta,\lambda) \tag{14}$$

then (12) implies that

$$\left|\bar{A}(\alpha,\lambda)\right|\le 1,\qquad \left|\bar{B}(\beta,\lambda)\right|\le 1 \tag{15}$$

or[5]

$$\left|\bar{B}(\beta,\lambda)\pm\bar{B}(\beta',\lambda)\right|+\left|\bar{B}(\beta,\lambda)\mp\bar{B}(\beta',\lambda)\right|\le 2 \tag{16}$$

Now consider

$$\begin{aligned}\left|E_\lambda(\alpha,\beta)\pm E_\lambda(\alpha,\beta')\right|&\le\sum_\lambda f(\lambda)\left|A(\bar{\alpha},\lambda)\right|\left|\bar{B}(\beta,\lambda)\pm\bar{B}(\beta',\lambda)\right|\\&\le\sum_\lambda f(\lambda)\left|\bar{B}(\beta,\lambda)\pm\bar{B}(\beta',\lambda)\right|\end{aligned} \tag{17}$$

where the second line follows from (12). Similarly,

$$\left|E_\lambda(\alpha',\beta)\mp E_\lambda(\alpha',\beta')\right|\le\sum_\lambda f(\lambda)\left|\bar{B}(\beta,\lambda)\mp\bar{B}(\beta',\lambda)\right| \tag{18}$$

[5] To show (16), consider the two possibilities $\bar{B}(\beta,\lambda)\le\bar{B}(\beta',\lambda)$ and $\bar{B}(\beta',\lambda)\le\bar{B}(\beta,\lambda)$ seperately.

Combining (16), (17), and (18) with[6] $\sum_\lambda f(\lambda) = 1$ we finally have

$$|E_\lambda(\alpha, \beta) \pm E(\alpha, \beta')| + |E(\alpha', \beta) \mp E(\alpha', \beta')| \leq 2 \tag{19}$$

But the quantum prediction does not always respect this inequality! Consider the measurement angles $\alpha = 0$, $\alpha' = \pi/2$, $\beta = \pi/4$, and $\beta' = -\pi/4$. Then, using the purely quantum mechanical expectation values from (10) gives

$$\left|E(0, \frac{\pi}{4}) + E(0, -\frac{\pi}{4})\right| + \left|E(\frac{\pi}{2}, \frac{\pi}{4}) - E(\frac{\pi}{2}, -\frac{\pi}{4})\right| = 2\sqrt{2} \tag{20}$$

where I have suppressed the subscripts for brevity.

People have performed this experiment and found that the experiments violated the Bell Inequality (19). This rules out the possibility that quantum mechanics is simply our best guess at an underlying theory which has a purely local explanation for the correlations observed in the EPRB experiment. It's also one of the best pieces of evidence that there is no deeper theory. People still work at finding loopholes in this argument, but quantum mechanics is looking strong!

Quick Question: Can you spot a way to create an underlying theory for which the derivation of (19) would not be valid?

2 Entropy

You may have heard of entropy in a chemistry class or possibly even in a physics course. Entropy was originally introduced in a field of classical physics known as *thermodynamics*. The concept was introduced around the 1850's, and is now immortalized in two of the famous laws of thermodynamics. The second law of thermodynamics tells us that perpetual motion machines are impossible because entropy is almost always increasing.

When I first learned about entropy, it seemed mysterious and arbitrary. Classically, it was defined in terms of heat transfer and temperature. These days, entropy is often introduced as a measure of disorder or chaos. But how do we measure disorder? A true understanding of this issue requires an understanding of quantum mechanics. Luckily, you now have that understanding!

Statistical mechanics is the field of physics which applies the ideas of quantum mechanics toward understanding thermodynamics. For very large systems in every day life, we don't care so much about the properties of a single particle. Instead, we study macroscopic properties such as energy, temperature or volume. Fundamentally all of these properties are consequences of the quantum state, but we discard much of that information in order to gain a useful understanding.

[6]This equality holds because $f(\lambda)$ is a probability distribution.

Typically, many different microscopic configurations correspond to the same values of the macroscopic observable. Let's look at a toy example. I'll spare you from the pains of dealing with a million particle state vector or having to ensure that such an object has the proper spin statistics. Consider a system of five distinguishable spin 1/2 particles. One possible microscopic state is

$$|\psi\rangle = |\uparrow\uparrow\uparrow\uparrow\downarrow\rangle \tag{21}$$

For a large system, one might only be interested in the total spin projection equal to the sum of all the single particle S_z values. The state in (21) has four up spins and a down spin to give $3\hbar/2$. But there are four other microscopic states with the same total spin projection!

Quick Question: Give another such state.

We define the entropy[7] to be

$$S = k_B \sum_i P_i \log P_i \tag{22}$$

The sum is over all microstates consistent with the macroscopic variables (in this case total spin) and P_i describes the probability that the system is in any individual state. Remember that physicists almost always mean the natural logarithm, i.e. $\log e^x = x$. For the example (21) we'll just assume that all states are equally likely. In this case we would find

$$S = k_B \sum_{i=1}^{5} \frac{1}{5} \log\left(\frac{1}{5}\right) = -k_B \log 5 \tag{23}$$

This suggests the more common Boltzmann style entropy, which is valid when all Ω microstates corresponding to the macroscopic description are equally likely:

$$S = -k_B \log \Omega \tag{24}$$

Quick Question: What is the entropy of the five particle system if the total spin projection is $5\hbar/2$? How about $-\hbar/2$?

One final word about systems like this one. If I put a bunch of spin 1/2 particles in a magnetic field, their energy is proportional to the total spin projection I have been discussing. Let's say $E \propto S_{\text{total}}$, ignoring constants and units. This system has zero entropy at the lowest energy (temperature), which is required by the Third Law of Thermodynamics. But it also has zero entropy at it's highest energy. For systems with this property, temperature[8] can actually be a negative quantity!

[7]This is called the Shannon entropy. Note that physicists use the Boltzmann constant and the natural logarithm. Computer scientists also use entropy, but they leave out k_B and use $\log_2$ to measure the entropy in bits.

[8]Temperature can be defined as the rate of change of entropy with respect to the total energy. In calculus notation this is $T = \partial S/\partial E$ where ∂ is a fancy kind of derivative.

3 Bose-Einstein Condensates (BECs)

We learned on day four about the difference between fermions and bosons. The requirement of antisymmetry makes it impossible for two indistinguishable fermions to occupy the same quantum state, but makes no such stipulation for bosons. In the 1920's, Satyendra Nath Bose was exploring the consequences of statistics for photons and discovered a strange prediction. At low temperatures, all of the particles in a system of bosons will occupy the same lowest energy state[9]. He sent his work to Einstein in a paper, which Einstein translated from English to German and championed for publication.

What does low temperature mean? Let's follow what happens as we cool a system of bosons down. For thermal systems, statistical mechanics tells us that states are distributed in states of different energy levels according to the temperature. At higher temperatures, more states are in higher energy levels. As we cool down a system, particles start moving towards lower energy levels.

For a system of N fermions, these eventually fill the lowest N energy levels of the system. Statistics prevents them from all sharing the same state. With bosons, there is a relation between a critical density and a critical temperature,

$$n_C = \zeta(2/3)\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} \approx 2.61238\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} \tag{25}$$

$$T_C = \frac{2\pi\hbar^2}{mk_B}\left(\frac{n}{\zeta(2/3)}\right)^{2/3} \approx 3.31\frac{2\pi\hbar^2 n^{2/3}}{mk_B} \tag{26}$$

Here n corresponds to density, the $\zeta(2/3)$ is a strange irrational number that comes out of the math, and m is the mass of each boson. If we are at a given temperature and increase the number of particles in the system such that $n > n_C$, every new particle we add goes into the ground state. Equivalently, decreasing the temperature below T_C for a given density starts to force more and more particles into the ground state.

Because of the constants involved, it takes a very low temperature to achieve Bose-Einstein condensation. It wasn't until 1995 that the first Bose-Einstein condensate was created out of 2,000 rubidium atoms at a temperature of 170 nK. You'll learn more about how this was achieved this afternoon.

BECs posess two very interesting properties that have led many labs to study them. First, they behave collectively like a single giant quantum system. All of the weird quantum effects then occur at micrometer scales, which is pretty enormous! The second property is that they can be very accurately controlled. Physicists have used BECs to reproduce other systems of study, but with tunable properties so that the effects of slightly changing the material can be studied. This has been primarily of interest to condensed matter physicists.

[9]The lowest energy state of a quantum system is called the *ground state*.