A Brief Exploration in Statistics and Quantum Mechanics

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Introduction

Quantum mechanics has some probabilistic or statistical features that have been considered paradoxical or exotic; at least, this impression is frequently conveyed in introductory textbooks on the subject and when physicists produce informal explanations of quantum theory. No doubt specialists in atomic physics have a solid grasp of these issues and can at any rate agree to disagree about difficult points of theory and experiment. But the often idiosyncratic treatment of statistics and probability in quantum mechanics seems unhelpful to the student and the interested layperson: it may tend to exaggerate and mystify the real differences between the microscopic and the macroscopic worlds, suggesting that the two worlds have little in common with respect to methodology. In this paper I try to show that some of the statistical esoterica of quantum mechanics can be made more transparent by their very close analogies to several macroscopic topics.

On the other hand, quantum mechanics also involves philosophical questions about epistemology and the nature of reality --questions which, though raised in the context of the atomic world, are as old as metaphysics. “Does the Moon exist just because a mouse looks at it ?” Einstein’s incredulous query echoes the ancient debate between nominalists and realists. This brief essay can contribute little to the clarification of such venerable issues except perhaps to cite the opinion of a wise practitioner, Henri Theil (1971, p. vi): “It does require maturity to realize that models are to be used but not to be believed.”

Uncertainty principle I: an ubiquitous trade-off

An important task of physics is to describe and predict an object’s trajectory through time –a planet’s orbit or the path of a rocket. A trajectory is constructed from sequential measurements of an object’s position and momentum: where is it now, in which direction is it going, and how fast is it moving ? At the atomic level, the objects of interest include, for example, electrons and photons. However, Heisenberg’s uncertainty principle shows that the trajectories of these particles cannot be determined exactly. The more accurately one measures a particle’s position, the more error one introduces into the measurement of its momentum, and vice versa (Hannabuss 1997, p. 83-86; Rae 1996, p. 76-80). In quantum-mechanical notation, the one-dimensional version of this trade-off is concisely expressed as

$$\Delta x \Delta p_x \geq h/4\pi \ , \qquad (1)$$

where Δx is the standard deviation of the particle's position, Δp_x is the standard deviation of its momentum, h is Planck's constant, and π is the familiar mathematical constant. Equation (1) means that the product of the standard deviations of position and momentum has a lower bound greater than zero. Beyond some point, a smaller Δx is associated with a larger Δp_x and conversely. Since the magnitude of Planck's constant is not negligible on the subatomic scale, the uncertainty principle implies an unavoidable indeterminacy for the trajectory of any particular particle; its path must be described in probabilistic terms.

On the other hand, Planck's constant is insignificant on a macroscopic scale, so the trajectories of planets and rockets can in practice be predicted with an accuracy limited only by the apparatus of measurement and observation. Therefore physicists frequently assert, in pedagogical and popular expositions, that the uncertainty principle has no application beyond quantum mechanics. Irving Kristol (1994) may perhaps speak for many physicists when he says, "Every time there is a major advance in physics or mathematics, some social scientists and humanists are quick to see in it a new paradigm for their own modes of thought. It was this way with Newtonian physics, Einstein's theory of relativity, the Heisenberg principle, and now chaos theory. All such 'trendy' efforts are soon revealed to be transient and foolish."

Nevertheless, the uncertainty trade-off is indeed implicit in many models that represent macroscopic phenomena in the natural and social sciences. For example, the covariance-stationary time-series models at the core of quantum mechanics are also used successfully in many other fields. Consider the simplest case, a first-order autoregression for some variable Y:

$$Y_t = \rho Y_{t-1} + u_t \qquad , \qquad (2)$$

where for stationarity $-1 < \rho < 1$. The innovation u_t is white noise with expectation zero and variance σ^2. At any time t, the variable's "position" is just Y_t, and during any interval its "momentum" is simply $Y_t – Y_{t-1}$. The variance of position is

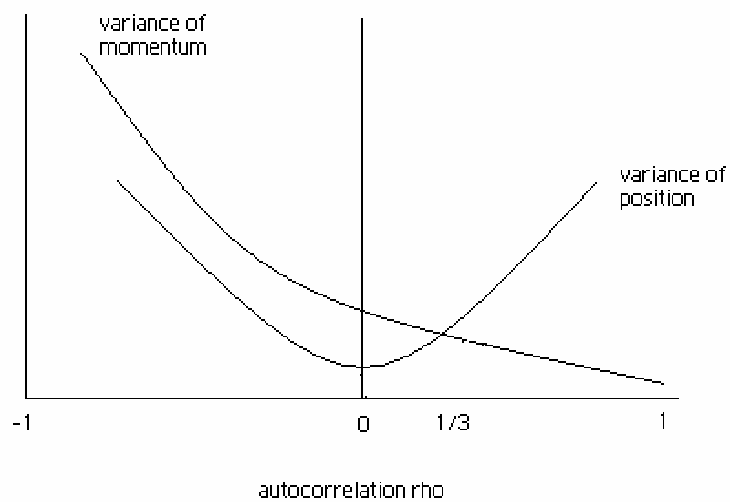
$$\sigma^2 /(1 – \rho^2) \qquad , \qquad (3)$$

and it is straightforward to show that the variance of momentum is

$$2\sigma^2/(1 + \rho) \qquad . \qquad (4)$$

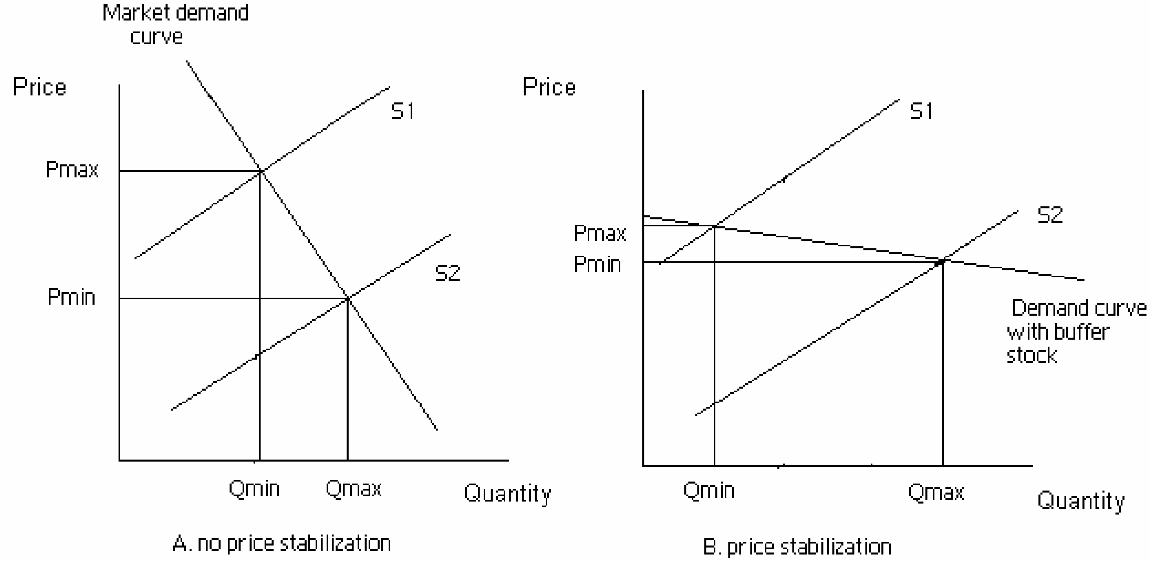
These expressions are graphed in Figure 1, where it is clear that both variances decrease as ρ increases from -1 toward zero. However, as ρ increases from zero, the trade-off emerges: the two variances move inversely. By analogy to equation (1), we minimize the product of (3) and (4) –or its logarithm-- with respect to ρ and determine that the lower bound is about $1.3\sigma^2$ when $\rho = 1/3$. Here the general scale parameter σ plays the role of h in equation (1). While Planck's constant is specific to quantum mechanics, σ has the dimension of Y, which depends on the context. Nevertheless, σ like h is supposed to be a constant; and like h it sets a bound on the accuracy with which the time path of Y can be known.

Figure 1. The uncertainty trade-off in first-order autoregression



As another instance of the uncertainty principle's appearance outside quantum mechanics, we remark that mathematicians and physicists have noted strong analogies between the Heisenberg trade-off and the Cramer-Rao minimum-variance bound that has a prominent role in linear statistical models (Frieden 1998, Stam 1959). Or we can cite examples from microeconomics that do not involve time series at all. If the government operates a buffer stock to mitigate the fluctuations of a commodity's price, is it an undiluted benefit for buyers and sellers ? Building on earlier work by F. Waugh and W. Oi, Massell (1969) analyzes this problem in a comparative-statics framework, a simplified version of which is shown in Figure 2.

Figure 2. Price stabilization and quantity destabilization



In the left-hand panel, the private market for an agricultural commodity is characterized by stable demand but unstable supply. The equilibrium price fluctuates widely between episodes of meager harvest (S1) and abundant harvest (S2) so the government creates a buffer stock to contain price movements within a narrow band around the average price. This is accomplished by buying for inventory when the price is below average and selling from inventory when the price moves above average; the effect of these operations is shown in the right-hand panel, where the demand curve is flatter (more elastic) than before the buffer stock. The range of price variation has indeed narrowed, but the range of quantity variation is much wider than in the private market. The government cannot stabilize the price without destabilizing the equilibrium quantities traded. Massell discusses the consequences of this trade-off for market participants.

Uncertainty principle II: it doesn't commute

Around 1925, when Werner Heisenberg was formulating the uncertainty principle, he collaborated with fellow physicists Max Born and Pascual Jordan, who recognized the matrix algebra underlying Heisenberg's work and recast the uncertainty principle in terms of "matrix mechanics." The scalar equation (1) can be replaced by its matrix counterpart:

$$P_X X - X P_X = (2\pi h/i)\mathbf{I} \quad , \qquad (5)$$

where P_X and X are respectively the momentum and position matrices, I is the identity matrix, and $i^2 = -1$. Unfamiliar with matrix algebra, Heisenberg was at first disconcerted that the matrix products P_XX and XP_X are not equal as they would be in the case of scalars. Today students of physics don't find non-commutating matrices perplexing, but the need for imaginary numbers may be puzzling; and in any case the standard treatment of (5) seems unnecessarily opaque.

Very simply, position and momentum are both modeled as stationary time series, so their cross-correlation matrix is asymmetric (Cryer and Chan 2008, p. 260-261): the correlation when position lags momentum by k time units is generally unequal to the correlation when momentum lags position by k time units. After all, if the two time series were monthly steel production and monthly auto production, would the correlation when autos lag steel by two months necessarily equal the correlation when steel lags autos by two months ? There is no reason to suppose so. This asymmetry accounts for the difference between P_XX and XP_X; and if the cross correlations are transformed from the time domain to the frequency domain, the imaginary unit i shows up because position and momentum are not "in phase" with each another.

Uncertainty principle III: time and energy

Related to the indeterminacy of position and momentum is another physical law called the "time-energy" uncertainty principle (Hannabuss 1997, p. 86-88), according to which a particle's energy can change abruptly during a brief time interval. The shorter the time interval, the greater the energy change can be. An electron may occasionally penetrate a barrier that it would normally find impassable; still one cannot say that the electron has violated an energy conservation law, for the instantaneous "tunneling" does not permit even a virtual measurement.

Suppose that Y in equation (2) is the price of a financial asset such as an exchange rate. Modern financial markets often use high-frequency data, including data collected in real time. As the discrete time interval in (2) shrinks toward zero, the autocorrelation ρ must approach 1; after all, the time series can change very little during an instant. It follows from (3) that Y's variance ("energy") is exploding. Y is transitioning from a stationary process to a process with a unit root –a random walk in the parlance of finance, Brownian motion to physicists. The statistical properties of economic and financial time series with $\rho \approx 1$ have been studied intensively during the last three decades (Phillips 1992; Cryer and Chan 2008, chapter 5).

The collapse of the wave function

In the 1920s**,** Heisenberg was not the only physicist unfamiliar with matrix algebra; many of his colleagues found the new mechanics uncongenial. They were more at home in the frequency domain and welcomed Erwin Schödinger's equivalent formulation in terms of a "wave function." Indeed, any stationary stochastic process indexed on time t has a unique power spectrum (i. e., variance) indexed on frequency f; by definition, t = 1/f. For example, the first-order autoregression in equation (2) has the power spectrum

$$2\sigma^2/(1+\rho^2 - 2\rho\cos(2\pi f)) \qquad (6)$$

for frequencies between 0 and ½ cycles per time period. If ρ is not much smaller than 1, the autoregression's variance is concentrated at low frequencies; if ρ is close to -1, then high-frequency variation is dominant.

The "dear radioactive ladies and gentlemen" (Pauli 1930) were probably happy to be at work again in the familiar domain of frequency, but an unpleasant surprise awaited them: the squared amplitudes of the Schrödinger equation do not correspond to actual waves at all but are instead probability densities as required by the uncertainty principle. For some physicists, that was a bridge too far. For example, how is the "collapse of the wave function" to be understood? The concept, inscrutable if one adheres to the notion of a physical wave, has a straightforward interpretation in terms of statistical sampling. While an experiment is being conceived and designed, several outcomes –perhaps many outcomes—are possible; and they can often be summarized by a probability density, e. g., the wave equation's squared amplitudes. Once the experiment has been performed, the *a priori* probabilities no longer apply to that particular experiment because its outcome has been ascertained; the wave function has collapsed. Speaking carelessly, a researcher might say, "In my data set, the 95-percent confidence interval is the sample mean ± 5 centimeters, so there's a 95-percent probability that the population mean falls in that range." Not so. The experiment has been performed, the sample has been drawn, the wave function has collapsed to either 1 or 0: the population mean, although unknown, is either in the interval ū ± 5 cm or it is not. [However, it is correct to assert that the population mean falls within the computed interval for 95 percent of a *large number of random samples (experiments)* having the same number of observations.]

Bell's inequality

This issue "goes back to Einstein, who was never happy with the primacy of statistical laws in quantum theory. In 1935, in collaboration with Boris Podolsky and Nathan Rosen, he discovered one of the most puzzling paradoxes of the theory, which exhibits very clearly the grounds for his unease. The paradox relies on the fact that conservation laws often provide information about one part of the system in terms of another. For example, if a stationary atom spontaneously decays into two fragments, their momenta must be equal and opposite. Measuring the momentum of fragment A tells us the momentum of fragment B as well. This suggests that we might be able to beat the uncertainty principle by measuring the position of B and the momentum of A. Combining the information would give both the position and momentum of B" (Hannabuss 1997, p. 167), the so-called EPR paradox.

However, Neils Bohr and his colleagues argued that "the system" cannot be separated into parts: the wave equation pervades the system, and its collapse due to a measurement at one point simultaneously impacts the other particles; they are "entangled." Einstein responded that such interactions across big distances (on an atomic scale) are counterintuitive, "spooky," and reminiscent of discredited notions like the luminiferous ether. He concluded that quantum mechanics is "incomplete" and conjectured that there might be "hidden variables" of which physicists are still unaware. Naturally, Einstein argued that realism requires such hidden variables to act locally, not spookily.

Subsequently, David Bohm proposed a thought experiment that applies an EPR-type strategy not to position and momentum but instead to the intrinsic angular momentum (spin) of a photon, which is characterized as being either up (+) or down (-). "An atom of calcium is irradiated by two lasers which excite it to a state of higher energy. It subsequently decays back to its original state emitting two photons of wavelengths 551.3 and 422.7 nanometers, respectively. Since the angular momentum of the initial and final states is the same one can show that the two photons emitted in opposite directions are identically polarized….By putting polarizing filters in the paths of the two photons one can find the correlations between them…." (Hannabuss 1997, p. 170).

Quantum theory produces an expression for the correlation between the two photons, but a different expression is implied by theories that satisfy Einstein's criteria for realism. Both theoretical correlations are functions of the angle at which the polarizing filter is set. J. S. Bell produced a theorem showing the polarizing angles at which the quantum-mechanical correlation and the "realistic" correlation would differ the most. The theorem involves an inequality which, if violated by the experimental data, is considered to be evidence in favor of the quantum theory and against the realistic theory.

An experiment consists of generating many photon pairs and computing their correlation. This process is repeated for a series of polarizing angles between 0 and π, the angle being set after the photons have moved apart "so that the second photon would pass through its polarizing filter before any signal could arrive (even at the speed of light) to reveal which polarization direction had been chosen for the first filter. In this way direct communication between the photons could be ruled out" (Hannabus 1997, p. 171-172); and Einstein's local hidden variables could not be invoked to explain violations of Bell's inequality.

The inequality has generated intense interest not only from physicists and mathematicians but also among philosophers of science and even in pop culture. Since the 1970s, Bell's inequality has been subjected to numerous experiments of increasing sophistication; and with few exceptions the inequality is violated, which has been interpreted as a vindication of quantum theory. It remains the case, however, that the efficiency of the experiments is often low: only 5-30 percent of the photons pairs are actually detected at *both* polarizing filters, the requirement to compute the relative frequencies.

Khrennikov (2008) has recently pointed out that Bell's inequality was known to mathematicians beginning with George Boole in the mid-nineteenth century. Of course, Boole and other mathematicians did not study the inequality in the context of quantum mechanics; instead they viewed it as a necessary condition for the existence of a single probability measure for the random variables. Violation of the inequality would mean that the probability space is not defined: for some values of the random variables, there would be negative probabilities, which are inadmissible. [Khrennikov (2008, p. 1457) comments briefly about the appearance of such anomalies in actual tests of Bell's theorem.]

Khrennikov then summarizes the situation from a probabilist's perspective: "We note that our considerations do not imply that the traditional interpretation of Bell's inequality…should be rejected. In principle, Bell's conditions (nonlocality, "death of reality") can also be taken into account. Our aim is to show that Bell's conditions are *only sufficient but not necessary* for a violation of Bell's inequality. Therefore, other interpretations of the violation of this inequality are also possible. Bell's alternatives, either quantum mechanics or local realism, can be extended: either the existence of a single probability measure for incompatible experimental contexts or quantum mechanics. We note that the existence of such a single probability was never assumed in the classical (Komolgorov) probability theory, but Bell used it to derive his inequality.…The question arises why we should use such an assumption in quantum physics although we have never used it in the classical probability theory.…We emphasize that for mathematicians consideration of Bell-type inequalities did not provoke a revolutionary reconsideration of the laws of nature. The joint probability distribution does not exist simply because those observables cannot be measured simultaneously" (Khrennikov 2008, p. 1448, 1450).

In terms of Bohm's version of the EPR experiment outlined above, Khrennikov argues that Bell erred in defining a single probability space for the entire apparatus; instead, a distinct probability space should be specified for each of the polarizing filters, which has its own operating characteristics and statistical variability. "In contrast to Bell, Boole would not be so excited by evidence of a violation of Bell's inequality in the EPR-Bohm experiment. The situation where pairwise probability distributions exist but a single probability measure cannot be constructed is rather common" (Khrennikov 2008, p. 1451).

"The consequences of the modern interpretation of the violation of Bell's inequality for the foundations of quantum mechanics…are really tremendous. Hence, the conditions for deriving this inequality should be carefully checked" (Khrennikov 2008, p. 1449).

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