ERIC R. SCERRI

THE EXCLUSION PRINCIPLE, CHEMISTRY AND HIDDEN VARIABLES

ABSTRACT. The Pauli Exclusion Principle and the reduction of chemistry have been the subject of considerable philosophical debate, The present article considers the view that the lack of derivability of the Exclusion Principle represents a problem for physics and denies the reduction of chemistry to quantum mechanics. The possible connections between the Exclusion Principle and the hidden variable debate are also briefly criticised.

The main purpose of this article is to consider the suggestion made by P.J. Hall (1986) that chemistry cannot be said to have been reduced to quantum mechanics because the reduction also requires the use of the Pauli Exclusion Principle which cannot be derived from quantum mechanics. Hall quotes Pauli himself, who as late as 1945 was still lamenting the fact that he had not been able to derive his principle from quantum mechanics.

I believe that there are far better reasons for denying that chemistry has been reduced to quantum mechanics as I have discussed elsewhere (Scerri 1991, 1994) and I also believe that Hall is mistaken in attaching any importance to the lack of derivability of the Exclusion Principle from Quantum Mechanics.

Hall claims that chemists differ from physicists in not being unduly perturbed by the lack of derivability due to the utility of the Pauli Exclusion Principle. However, apart from the Pauli quotation Hall is unable to offer any evidence of physicists being concerned over this issue. Hall merely states,

> discussion of this difficulty does not appear to be currently fashionable. (Hall 1986, p. 270)

One can only conclude that if physicists were ever perturbed by this question, this has ceased to be the case and consequently this cannot be held to be a difference between chemists and physicists. Furthermore, I wish to argue that this alleged lack of derivability does not in fact represent a difficulty for physics.

Of course it would be desirable to have a theory which could explain why only anti-symmetric wavefunctions apply to fermions. However I do not believe that we are justified in expecting a derivation of the

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Pauli Exclusion Principle from present-day Quantum Mechanics. My reason for saying so is that I regard Quantum Mechanics and the Pauli Exclusion Principle as inhabiting different epistemological levels. Quantum mechanics is a general theory which governs all types of particles. However, the Pauli Exclusion Principle only applies to fermions, or half-integer spin, and places a restriction upon their behaviour, namely the anti-symmetry of the wavefunction. It does not place this restriction on bosons or integer-spin particles. It is unreasonable to expect *any* restriction to be derived from general principles.

What Pauli did achieve, and which Hall does not seem to be aware of, was to show a connection between statistics and spin (Pauli 1940, 1941). Pauli established this connection by, in a sense, ruling out the wrong connections. He showed that it is not possible to achieve a consistent quantisation of an integer-spin system by Fermi statistics and equally impossible to quantise a half-integer system by Bose statistics.[1] For example, a half-integral spin system contains negative energy solutions. If this system is quantised by Bose statistics the exclusion principle is not available to fill the negative energy sea. The result is the unacceptable feature of a Hamiltonian which is not bounded from below.[2]

Hall also makes the following remarks about the Exclusion Principle,

> . . . it was not until after Dirac's work on relativistic quantum mechanics and the theoretical statement of electron spin that it was fully fitted into the framework of quantum mechanics and formulated as the Antisymmetry Principle. (Hall 1986, p. 268)

I believe that Hall is committing two errors in this statement. First of all, he seems to contradict the main thrust of his own paper when he says that the Exclusion Principle was *fully* fitted into the framework of quantum mechanics. Secondly, it was simply not the case that the quantum mechanical formulation of the Antisymmetry Principle had to await Dirac's relativistic treatment of the electron. The quantum mechanical version of the Exclusion Principle was first given by Heisenberg in 1926 (Heisenberg 1926) and was independently rediscovered by Dirac (1926) a full two years before his relativistic paper (Dirac 1928). Dirac's relativistic treatment of the electron predicted spin and not the Exclusion Principle.[3]

Another inaccuracy in Hall's account occurs when he suggests that as a result of the Exclusion Principle,

> . . . . as successive electrons are added to a nucleus they are forced into higher and higher energy states as the lower states are fully occupied.

This feature does not result from the Exclusion Principle but was already inherent in Bohr's Aufbauprinzip. Through the Exclusion Principle, Pauli did not claim to explain the fact that additional electrons are forced into higher and higher energy levels but only claimed to explain the length of each period.

Having already argued for a certain 'incompleteness' in the theory due to the alleged uneasy marriage between Quantum Mechanics and the Exclusion Principle, Hall then makes a huge leap to present issues in foundations of quantum mechanics. He asserts that any future theory which might be capable of predicting the antisymmetry of the wavefunction would "tie up with the rest of the hidden variable debate", although this is not explained further. He also claims that this new theory would describe an "extra dimension" and that this interaction would involve spin. The following three, neither necessary nor sufficient reasons, in my view, are then given to support this idea (Hall 1986, p. 271–2).

(1) The Exclusion Principle ultimately reduces to a spin effect. The effect on other orbital quantum numbers follows from this.

(2) The Aspect experiment rejection of local hidden variables can be explained by and is concerned with an interaction between spins of particles.

(3) Popper seems to express an important truth when he says:

> First we know so little about spin that it could be that Bohm is mistaken in supposing that his version of EPR, relating to spin, is essentially equivalent with the form proposed by Einstein. (Popper 1982, pp. 23–4)

Starting with point (1), it is difficult to see what is intended by the second clause. What is supposed to be the effect upon the other three quantum numbers which follows from the Exclusion Principle?

Point (2) contains a serious factual error. The Aspect experiment is not concerned with the spins of particles but with photon polarisation. It is not essential to measure particle spin to test the validity of hidden variable theories.[4]

In his point (3) Hall succeeds again in contradicting himself, since if Popper is indeed correct, then the fundamental connection between electron spin and the EPR/hidden variables work which Hall wants to make would collapse.

To conclude, I do not believe that the connections which Hall has tried to draw between the Exclusion Principle and the current debate in foundations of quantum mechanics are valid. This is not to say that such a connection, perhaps along the lines suggested by French and Redhead may not be possible (French, Redhead 1988; French 1989).

NOTES

[1] Nevertheless, Pauli did revisit this question on several occasions. For example in 1955 he returned to the problem in order to generalise the theorems to include fields as well as free particles (Pauli 1955).

[2] There is also an informal connection between quantum mechanics and the indistinguishability of particles since the uncertainty principle prohibits the following of a trajectory of any individual particle.

[3] The first person to consider the notion of a spinning electron was Kronig who on consulting Pauli on the subject was so severely criticised that he decided not to publish his views (Kronig 1960). Electron spin was eventually introduced by Uhlenbeck and Goudsmit who took the precaution of not consulting Pauli for his opinion (Uhlenbeck and Goudsmit 1925) Pauli continued to reject the notion until he was finally convinced of the usefulness of spin by the calculations of L. H. Thomas (1927). Interestingly, it later emerged and it is now generally agreed that the term electron spin is something of a misnomer since the electron does not strictly behave like a spinning object (see for example, Atkins 1983, p. 115).

[4] Bell's inequality can also be tested through two-photon interferometry, which uses directional correlation of photons rather, than polarisation correlation (Rarity et al., 1990). I am grateful to an anonymous referee for pointing this out.

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Centre for Philosophy of Natural and Social Sciences
London School of Economics
London WC2A 2AE