Research News

Gauge Theory – A New Outlook on Solid State Dynamics

By Stanley Clough *

Occasionally in science a new outlook arises which radically changes perceptions and genuinely deserves the overworked description "breakthrough". Such an event has occurred recently in the recognition of the fact that the dynamics of condensed matter must be described by gauge theory.[1-3] A consequence has been to throw new light on the hitherto dark and mysterious relationship between the quantum and classical descriptions of solid state dynamic processes. A sound basis is provided for classical models and attention is now focused on new phenomena which can be expected when neither pure quantum nor pure classical descriptions are appropriate. The most important consequence however, is that the incorrect procedure and concepts which have been commonly used are highlighted.

One of the problems about understanding the properties of materials is the need to choose either a quantum mechanical or classical description, when the relationship between the two descriptions can be quite obscure. This is in spite of the existence of phenomena which are clearly quantum mechanical at low temperature but better described classically at high temperatures. A hybrid theory which would encompass both regimes has never existed. Its non-existence has even been part of a dogma which insists that only the mysterious Copenhagen interpretation links the two types of theory. It is as if we had to use two different languages in the north and the south of a country with no guidance about what to do in the middle. Nature, we were told, is like that. Now it appears that nature is more sensible. We were leaving out key features called symmetry breaking and *Berry*'s phase. Now the two languages are revealed as different dialects of the same language and one merges smoothly into the other. The hybrid theory that spans both quantum and classical regimes exists. It is gauge theory.

Berry's discovery was that there are two ways in which the phase of an eigenfunction can advance, not one as previously supposed. Quantum mechanics had been structured to handle the motion of one system but not two, and the phase associated with one system driving another had been overlooked. Not for the first time, science had mistaken a special case for the general one. The analysis of most problems of condensed matter involves a decomposition of the whole sample into two parts, a subsystem whose motion is to be described and a thermal heat bath where the effect of the latter on the former is crucial to the description. Regarding the subsystem to be isolated leads to a set of eigenstates and eigenvalues for the subsystem with the latter controlling the evolution of the phase of the wave function. When the interaction with the heat bath is switched on, the state of the subsystem changes and a new way in which the phase of its wave function can change comes into play.

The idea which makes these statements tangible is symmetry breaking. In order to swim a spherical creature must deform to create a paddle. In the same way, the symmetry of an isolated system is broken when it interacts, and one or more new coordinates are created through the interaction. Symmetry breaking is a common occurrence throughout physics and is usually discussed by means of a schematic diagram like Figure 1. This represents a potential energy surface with the shape of the bottom of a wine bottle, i.e., a central maximum surrounded by a circular trough. Superimposed on the central maximum is a deep minimum which

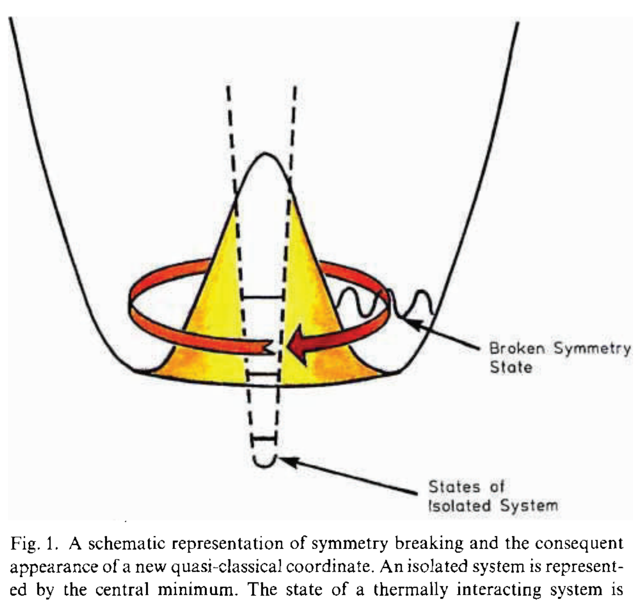

Fig. 1. A schematic representation of symmetry breaking and the consequent appearance of a new quasi-classical coordinate. An isolated system is represented by the central minimum. The state of a thermally interacting system is described by a wave packet in the circular trough, combining both quantum and quasi-classical features, the latter arising from the *Berry*'s phase associated with motion around the trough.

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represents the isolated system with its set of energy levels. When the interaction with the surroundings is turned on, the symmetry breaks and the wine bottle potential comes into play. The state of the subsystem is now a wave packet located in the circular trough and the new coordinate generated by the interaction is the position in the trough. The interacting environment drives the wave packet around the trough and this is the motion which leads to the acquisition of *Berry*'s phase. The dynamics therefore require specification of the wave packet as a linear combination of the states of the isolated system, and also the driven motion around the trough. At high temperatures the wave packet is a mixture of many states of the isolated system, averaging out the quantum motion, and the wave packet becomes localized so that its motion in the trough acquires a classical particle-like character. In this way there is a smooth progression from the almost pure quantum behavior of a weakly driven system at low temperature, when the energy levels determine the dynamics, to the quasi-classical behavior of a thermally driven system at high temperature. In the light of this description it is easy to see how earlier discussions, which attempted to describe the temperature dependence only in terms of the states of the isolated system (being unaware of the symmetry breaking, the motion associated with the new coordinate(s) and *Berry*'s phase) were handicapped.

The history of gauge theory and how it finally arrived in solid state physics is an interesting story. Its origin is the most radical idea of the century, *Einstein*'s geometrization of gravitation in his theory of general relativity. *Newton*'s force of gravity was replaced by a curvature of space into time. The notion that other forces might be represented (or replaced) by curved spaces was immediately taken up by *Weyl* in 1919 in the first gauge theory which was an example of an idea before its time. Its somewhat unhelpful name dates from this period. The problem was that no other space could be imagined into which the xyz space could be curved. It was not until the advent of quantum mechanics, when the phase of a wavefunction could be identified as a kind of additional particle coordinate in an intangible "internal" space, that the nature of the curvature in *Weyl*'s theory could be recognized. Two sub-spaces may be said to be curved into each other if a displacement through one entails a shift in the other. Thus moving a clock in a gravitational field results in a change of its time rate because space-time is curved. The gravitational field determines the magnitude of the effect and is a measure of the curvature. Similarly, a quantum particle moving in a region in which the external xyzt space time is curved into the "internal" space, experiences a change in the internal coordinate, i.e. the phase of the wave function. This provided a brilliantly simple description of electromagnetism and the foundation for particle physics theories. However, gauge theory became associated with the intangible "internal" spaces and its application to the more mundane problems of condensed matter was overlooked.

The wave function of a charged particle moving through a space–time vector dr experiences a phase change q $(A.\ dr)$ where A is the electromagnetic vector potential. Thus electromagnetism can be recognized as a gauge theory arising from the existence of a very simple internal charge space. The six components of the electromagnetic field, E_x, E_y, E_z, B_x, B_y and B_z represent the curvature of the internal space into xyzt measured in the planes xt, yt, zt, yz, zx, and xy, respectively. The internal charge space is experienced only by particles carrying electric charge and can be visualized as a circle of values between 0 and 2π. All electromagnetism follows from this. The curvature is due to the presence of other charges, so that the interaction between charges occurs as each charge modifies the curvature of the space through which other charges move.

The elaboration of the theory for more complex internal spaces laid the foundation for theories of the nuclear forces between fundamental particles, which resulted later in the spectacular successes of the electro-weak theory for the unified electromagnetic and weak nuclear interactions, and quantum chromodynamics for the strong interaction. In these theories the curvature is quantized with the appearance of exchange particles like the photon in electromagnetism. A further element in the argument was required to account for the mass of the exchange particles associated with the weak interaction. This crucial element is symmetry breaking.

Solid state physics remained largely isolated from these developments of the 60's and 70's. There were warning signals that it had adopted some false concepts, but there were also standard explanations which covered up the contradictions. Then in 1984/5 the term *Berry*'s phase (or the topological phase) began to be heard and to become very common in titles in Physical Review Letters. *Berry*'s innovation [1] was to consider the evolution of the wave function of a driven system rather than a dynamically isolated one. He showed that it acquired an extra phase (*Berry*'s phase) dependent on the geometry of the driven trajectory. *Simon*[2] saw at once that this phase was a consequence of the trajectory of the driven system occurring on a curved space, and *Wilczek* and *Zee*[3] recognized the mathematical structure of gauge theory. It had finally arrived in solid state physics.

It should have been no surprise. Most problems in the solid state require a division into a subsystem P and its thermal environment Q. If subsystem P drives subsystem Q then the coordinates of the two subspaces P and Q cannot remain pure. The spaces are curved into each other and the curvature replaces the forces which each exerts on the other. Space Q acts as an "internal" space for P, and vice versa. The interaction of such systems is described by gauge theory. This means that the differential momentum operator $\partial/\partial x^P$ is replaced by the covariant derivative $D = ((\partial/\partial x^P) + iA)$. This is the prescription for differentiating on a curved x^P surface. A is a vector potential which describes (through the derived field) the curvature of the surface. It depends on the state of the interacting subsystem Q and therefore allows one subsystem (the heat bath) to drive the other (the system under examination). The curvature introduced by the interaction changes the space of the isolated system and is responsible for symmetry breaking.

The story so far can be summarized by saying that gauge theory is the universal description for forces between interacting systems. To understand its importance for condensed matter science, it is necessary to appreciate the bad state the latter has fallen into because of the lack of awareness of curvature. Briefly, solid state physics exists in curved spaces which have been treated as flat. Some of the consequences of curvature have been introduced in an ad hoc way and some left out. Naturally this has caused confusion. The confusion has been concealed by a set of concepts which have been developed to make physical sense out of false theoretical structure. Gauge theory with symmetry breaking blows away this conceptual smoke-screen and replaces the rather abstract mysteries by a much simpler set of ideas.

The simplest example of solid state dynamics which illustrate these matters is the hindered rotation of symmetrical molecular groups like CH_3 or NH_4 in crystals. At low temperature these exhibit clear quantum mechanical tunneling motions and at high temperatures their rotation can be described in terms of classical hopping between the wells of the hindering potential. The discrete quantum phenomena at low temperature can be accounted for by the cyclic boundary condition $\psi(\Phi) = \psi(\Phi + 2\pi)$, where Φ is the rotation coordinate. This is normally justified by the statement that the wavefunction must be single valued. In fact it only applies to the special case where the group is dynamically isolated. If it interacts with the environment so that the two move together in a correlated way then the boundary condition takes the form $\psi(\Phi) = \psi(\Phi + 2\pi)\exp(iy)$ where y is connected with the movement of the environment. The phase factor y is *Berry*'s phase and for a methyl group it is connected with the thermally activated rotation rate. At low temperatures y is small and the effect of the boundary condition is to allow only a small number of rotational states. For the methyl group these are three in number known as A, E^a and E^b, the latter pair being degenerate. The energy difference between the A and E levels is the tunnel splitting. This determines the frequency whose reciprocal specifies a time during which an additional phase y is acquired. At higher temperatures the root mean square value of y grows. When it is of the order π, the boundary condition has lost its restrictive character and a broad band has replaced the discrete levels. In short, thermal broadening has occurred clearly related to the rate of driven rotation. The magnitude of the broadening becomes identifiable as the reciprocal of the correlation time for the driven rotation as assumed in purely classical theories.

The intervention of the environment in defining $\Phi + 2\pi$ relative to Φ curves the one dimensional Φ space which may be regarded as being changed from a flat circle into a helix. This symmetry breaking is the key to an understanding of how classical mechanics can emerge from quantum mechanics. Symmetry breaking is an inevitable consequence of interactions, as for example, when two previously spherical atoms form a chemical bond. Methyl rotation is just the simplest example but the conclusions apply quite generally. The effect of the environment breaks the symmetry of the isolated system, introduces new coordinates which are embryonic versions of the classical ones, and as the fluctuations of the environment come to dominate, a smooth transition from quantum to classical behavior occurs.

How has solid state physics managed so long without these concepts? Without the broken symmetry and its quasi-classical coordinate and associated *Berry*'s phase, the attempt has been made to explain quantum damping or motional broadening only in terms of the levels in the central minimum of Figure 1. The observable broadening now attributable to *Berry*'s phase was wrongly accounted for by life time broadening of the levels due to incoherent transitions between them, though how the rate of thermal transitions between levels could be measured in thermal equilibrium was not explained. Since vibrational excitation clearly has nothing to do with rotation, it led to a curious doctrine of separation. This supposed there to be two kinds of concept, quantum and classical, and asserted that no theory should contain both. Thus rotation is a classical concept, along with torque, and according to this doctrine should not figure in a quantum theory. This made the absence of driven rotation into a principle, which was reassuring but wrong. In the central minimum there is no motion clockwise or anticlockwise because time-reversal symmetry remains unbroken, but the quantum motion can be described as a kind of bidirectional motion, both clockwise and anticlockwise simultaneously. It was then argued that the Copenhagen interpretation meant that the apparent bidirectional motion was to be interpreted statistically as either clockwise or anticlockwise rotation. This introduced rotation but it had nothing to do with the broadening and nothing to do with the lattice. Using such devices, a conceptual gap was concealed for many years. The new insights of gauge theory solve many problems simultaneously and carry the weight of established success in relativity, electromagnetism and particle physics. The new developments represent a long delayed achievement of a unified approach to interactions across the whole of Physics.

[1] M. V. Berry, *Proc. R. Soc. A392* (1984) 45.
[2] B. Simon, *Phys. Rev. Lett. 51* (1983) 2167.
[3] F. Wilczek, A. Zee, *Phys. Rev. Lett. 52* (1984) 2111.