ION BAND STATES: WHAT THEY ARE, AND HOW THEY AFFECT COLD FUSION

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It is not a difficult task to understand why cold fusion takes place. One needs only to think of it more in terms of the way transistors work than vacuum tubes work. We find it easy to visualize the operations of a vacuum tube, in which pointlike electrons are boiled off a hot filament to form a cloud of colliding objects that drift down an electric field onto a plate collector. This flow can be controlled by varying the potential on a negatively charged grid placed between the filament and the plate. But the physics of atoms, molecules, metals, and semiconductors cannot be described realistically with this type of thinking. In a transistor the electrons that are responsible for conductivity more closely resemble stationary waves than moving point particles. The energy of the electrons depends on the direction and amplitude of their wave vectors. The electrons occupy an energy band rather than a single energy state. Moreover, because of the Pauli exclusion principle, the set of electrons can completely fill an allowed band, in which case a semiconductor resembles an insulator. When the band is not quite filled, one has a p-type semiconductor, and when it is overfilled so that a few electrons have been forced to enter an otherwise empty band state, one has an n-type semiconductor. It is this interplay between periodic order, which allows electrons to be wave-like, and periodicity disruption (e.g. trapping sites), which allows electrons to be more particle-like, that controls the flow of current in transistors. Without this interplay and the ability to control electrons in this manner, there would be no modern day computers or solid state electronics.

The physics of Fleischmann and Pons (F and P) type cold fusion[1] differs from the physics of electrons in a solid because it deals with D^+ ions (deuterons), which do not obey the Pauli exclusion principle. These particles, like electrons, can occupy band states, as shown by Casella[2] and a number of other workers[3-5]. The important point is not the fact that band states can be occupied, but that D^+ ions occupying band states resemble stationary waves rather than point particles. Transistor type thinking applies. As in the physics of transistors, it should be possible to control cold fusion by controlling the behavior of the stationary waves that are responsible for the phenomena.

Quantum mechanics provides the means for describing the behavior of particles subject to different environments. The allowed behavior is embedded in the particle system wave function. The type of wave function that describes the behavior of a particle occupying a band state in a periodic solid is called a Bloch function, named after Felix Bloch. Bloch functions have the same spatial distribution in each unit cell of a crystal, with only the wave phase changing with position within the crystal. The active ingredient in F and P type cold fusion is Bloch function D^+, designated D^+_{Bloch}. Deuterium in D^+_{Bloch} form is as different from the interstitial D atoms normally encountered in metal deuterides as ozone O_3 is from molecular oxygen O_2.

An important aspect of cold fusion is that very little D^+_{Bloch} is required to release heat at the power levels observed by F and P, and others[6]. Reaction rate calculations[7] show that only about 10^{-7} D^+_{Bloch} per Pd atom may be required to give 600 W/cc. This reaction rate was calculated using the ordinary rules of quantum mechanics and using a nuclear potential *V* that is zero whenever the reacting D^+_{Bloch} don't occupy the same volume of space and whenever they don't have antiparallel nuclear spins. When overlap occurs with proper spin cancellation V = -23.8 MeV for the 2 $D^+ \rightarrow {}^4He^{++}$ reaction. Like the D^+, the ${}^4He^{++}$ must be in an overlapping band state. Nuclear physics allows no interaction at a distance, i.e. requires non-zero wave function overlap. Reaction rates are calculated by the Fermi Golden Rule of time-dependent perturbation theory[8]. The requirement for D^+-D+ overlap is the property that forces free particle fusion to occur only at high temperatures. This requirement for overlap also prevents D^+-D^+ fusion in D_2 molecules, and makes futile all attempts to achieve fusion by squeezing D atoms together inside a solid.

So why does D^+_{Bloch} fuse whereas the D_2 molecule is highly stable? The answer to this question goes back to the guiding rules of quantum mechanics as applied to bound state physical systems, i.e. the wave function must minimize energy. Physics says that the correct ground state wave function is the one that minimizes system (kinetic plus potential) energy. If the lowest energy is achieved with wave functions that keep the D^+ separated from each other, there will be no fusion, but if it occurs with the D^+ having overlapping wave functions (finite amplitude when separation distance r_{12}=0), then fusion is allowed. To keep the particles separated, the many-particle wave function has to decrease to zero at each 2-particle zero-separation distance. The deviations in the wave function that are required to do this cause increases in kinetic energy. As a result, in some systems, minimum energy is achieved without full particle avoidance. For example, as shown in Fig. 1, the two electrons of the helium atom have more than 70% overlap[9] (most of the time), hence would undergo fusion if they had the nuclear properties of deuterons. But when the mass of the particle is larger, the kinetic energy increase associated with the same amount of wave function curvature is reduced. Because of the heavier deuteron mass, the D_2 molecule, which has the same order of size as the helium atom, has minimum energy with zero D^+-D^+ overlap.

Fig. 1 Amplitude squared of the helium ground state 2-electron wave function on the surfaces of 2 spheres of constant radius (=s/2). Values have been normalized with respect to the peak values, which occur when the 2 electrons are on opposite sides of the nucleus (θ=180○). Nature uses a cusp (a pointed dimple) when separation r_{12} = 0 to compensate for the infinite electrostatic potential existing at this condition. The amplitude squared at $\theta=0^\circ$ measures the degree of electron-electron overlap. The electrons spend most of their time at s<0.5 Bohr radius. If the electrons had the nuclear properties of deuterons, they would fuse.

But what about a metal containing D^+_{Bloch}? Here the answer depends on host crystal size, i.e. the volume V_{xtal} over which the stationary wave description is valid[10]. When the crystal is very microscopic, the system resembles the D_2 molecule. There is no overlap and no fusion. But when the crystal is of the order of 0.4 micron in size, the overlap is essentially complete and the behavior resembles that of the electrons in the helium atom. This change in overlap in the ground state wave function is a result of the different behavior of the kinetic energy relative to the potential energy when the many-body wave function amplitude goes to a minimum at zero D^+-D^+ separation. The potential energy decrease varies as $1/V_{xtal}^2$ whereas the kinetic energy increase varies as $1/V_{xtal}$ for the case where the ion charge is shielded by a neutralizing electron cloud within the volume of one unit cell. For crystals larger than about 0.4 micron, kinetic energy dominates over potential energy and the situation resembles that of the 2 electrons in the helium atom rather than that of the 2 D^+ in the D_2 molecule, i.e. there is D^+-D^+ overlap, hence fusion. The details of electron screening do not affect this general result.

The other big question is: Why is cold fusion radiationless? Here the answer is found in Fermi's Golden Rule of time-dependent perturbation theory[8].

$$w = 2\pi/\hbar^2\, |\langle k|V|s\rangle|^2\, \rho_£(E_k^{(O)}) \quad ,$$

where w is the reaction rate (transition probability per unit time), $\langle k|$ and $|s\rangle$ are the final and initial state wave functions of the total system, V is the perturbing potential, (in our case the nuclear potential), and $\rho_£(E_k^{(o)})$ is the density of final states of the unperturbed system Hamiltonian when final state energy $E_k^{(0)}$= initial state energy $E_s^{(o)}$. The states $\langle k|$ and $|s\rangle$ include not only the D^+ and $^4He^{++}$ Bloch functions, but also the lattice and its excitation spectrum. The nuclear reaction makes available in each unit cell $23.8/N_{cell}$ MeV energy, which is available for lattice excitation. N_{cell} is the number of unit cells in the crystal, which is typically $> 10^9$ for a 0.4 micron crystal. The large number of lattice excitation modes available to this energy makes the transition irreversible and prevents the energy from becoming concentrated into a single unit cell, as required for energetic particle emission.

With this background we can identify some of the research requirements for cold fusion. The experimental problem for F and P type cold fusion is: How do you create and contain a D^+ Bloch population within a metal or metal hydride? Fundamental to the ion band state picture is that energy be minimized in an environment in which there is sufficient periodic order. Just as in the case of electrons in transistors, it is the interplay between periodic order and disorder that dictates whether or not a D^+ Bloch population will exist. Previous theory[7] shows that a fully loaded PdD crystallite containing 10^8 unit cells should support cold fusion in which the energy is released in the form of long-wavelength phonons and never becomes concentrated so as to release energetic particles, and in which the product wave-like $^4He^{++}$ is released at the crystallite surface. The work of Storms[11] suggests that occupations of the band state increases with temperature, indicating that thermal excitation played a role in state occupation in his experiment. In the work of McKubre et al.[12] and Hasegawa et al.[13] the bulk D/Pd ratio serves both as a measure of the surface chemical potential achieved in their electrolysis operations and of the chemical uniformity produced in their cathodes. Their D/Pd ratios exceed those of equilibrium chemistry, suggesting that an D^+ ion transmitting polarized layer on their cathode surfaces created a potential barrier against ion escape for the Pd surface. This condition leads to a higher chemical potential within the bulk than would otherwise exist.

A competing approach to cold fusion uses ion implantation. With ion implantation there seems to be a need for full encapsulation of the reactor within a barrier layer that blocks passage of D_{+Bloch}. The D_{+Bloch} can be expected to have vastly different transmission properties than possessed by interstitial hydrogen. A very thick barrier layer, or one that destroys all periodic order, may be required. Ion implantation through this layer would be needed to create and maintain the D_{+Bloch} required for fusion.

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