THE ROLE OF HYDROGEN ION BAND STATES IN COLD FUSION

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Abstract

Quantum diffusion studies of hydrogen (H) and deuterium (D) inside and on the surfaces of transition metals indicate that both H and D may occupy wave-like band states (H and D ion band states) analogous to the electron band states that are responsible for making metals conductors. When these wave-like ion band states become occupied, fusion involving D+D→^4He without emission of gamma rays or other high energy by-products can occur, provided a number of conditions are met. We have previously identified and used these conditions to predict a number of important experimental results that were subsequently observed. In part 1 we examine the underlying justification for believing that ion band state occupation can lead to nuclear reaction. We show that under suitable conditions associated with the underlying electronic structure, ion band state occupation may lead to wave function overlap between a small number of indistinguishable D. These conditions appear to be met as x→ 1 in PdD_x. Then, ion-ion correlation effects that result from coulomb repulsion, which normally inhibit overlap, are not present in the ground state wave function, provided the number of indistinguishable ion band state deuterons is very much less than the total number (N_{cell}) of unit cells in the crystal, and the crystal is sufficiently large : N_{cell} > 10^8. In part 2, we examine the implications of the ion band state fusion scenario, including a summary of important selection rules and reactions which follow as a result of the restrictions that are implied by the physical limit in which the theory applies.

Introduction

Acceptance of cold fusion as a real phenomenon by the mainstream physics community has been delayed mainly for two reasons: 1) a refusal of physicists to believe that the coulomb barrier that normally prevents nuclear reactions at room temperature can be overcome in the solid state environment, and 2) a belief that γ-ray and high energy particle emission must inevitably accompany the release of nuclear energy. The cold fusion community for the most part bases its belief in cold fusion on the evidence for the reality of the cold fusion heat effect. Nonetheless, it shares with the larger physics community a belief that mainstream physics cannot overcome the coulomb barrier problem and cannot provide radiationless emission. This paper presents an alternate view, based on ordinary quantum mechanics, that
explains not only how the coulomb barrier can be overcome in a radiationless manner and why this can be done using the procedure developed by Fleischmann and Pons, but also why this procedure leads to unexpected products, modes of energy release, and other effects that have been observed. The underlying ideas behind this alternative view are closely tied to the known electronic properties and structure of palladium deuteride PdD, and the governing rules of bound (as opposed to unbound) systems, and known effects associated with periodic order and the exchange of identical particles.

In the resulting picture, cold fusion is the result of a relatively small number of D+ occupying wave-like (Bloch function) band states. Once this happens, as a result of the behavior of indistinguishable particles, these wave-like D+ ions are free to overlap each other and fusion can occur. An important point is that the D+ become delocalized as a result of occupying these states. The associated nuclear reactions also become distributed. This leads to different, distributed modes of interaction, in which the effects of periodic order and particle indistinguishability alter the relevant forms of reaction. From the underlying physics, it follows that in these distributed, transistor-like (as opposed to vacuum tube-like) modes of interaction, high energy particle and γ-ray emissions are not to be expected. Also, the underlying assumption that D+ ion band state occupation should occur becomes valid in the limit that x→1 in PdDx.

In the paper, we first examine what we believe to be the most compelling experimental evidence in support of excess heat. Then, using a concrete example, we explain the underlying logic, based on system energy minimization, behind our conclusion that the quantum mechanics of bound systems can potentially alter particle-particle overlap in a manner that may significantly affect the possibilities for nuclear reaction. We also explain why energy minimization precludes the possibility of nuclear fusion between chemically bound D or in D2 molecules, but that the same principle can be used to demonstrate that under suitable circumstances nuclear reaction can occur between D+ ions within a sufficiently large, periodically ordered solid as a result of ion band state occupation. In the remainder of the paper we examine the underlying implications and conditions associated with ion band state occupation and interaction, including a summary of the important restrictions and selection rules associated with potential ion band state mediated nuclear reactions.

I. Underpinnings of Excess Heat Cold Fusion Theory

Evidence for Excess Heat

Before exploring the theoretical aspects of cold fusion, we briefly consider the evidence for the reality of cold fusion heat. There have been many observations of excess heat in electrochemical system experiments. Among the hardest to refute are the observations of Fleischmann and Pons during temperature excursion events in which water in their electrolytic cell boils away. The energy balance observed in their temperature-increase event published in Phys. Lett. A is:
• Heat of vaporization of 47 cc D$_2$O: 102500 J in 10-minute boil-dry period
• Concurrent electrolysis power input: 22500 J
• Missing heat (cold fusion): 80000 J

The missing heat corresponds to 197 eV per Pd atom, which exceeds by a factor of 20 the value possible from stored chemical energy. The only mainstream physics possibility is that the heat was derived from the nuclear potential.

Why Ion Band State Matter Avoids the Coulomb Barrier: Guiding Principle
There is considerable common ground among physicists concerning the principles of physics, and the requirements of a successful theory of the cold fusion heat effect. A successful theory must explain how the coulomb barrier is overcome and why fusion is radiationless. For nuclear reaction to occur there must be wave function overlap of the feedstock components and also wave function overlap with the product. There is also agreement that in free space this overlap can be explained by scattering theory, which provides transient overlap calculable from Gamow theory. On the other hand there does not seem to be an equal acceptance as to how one properly proceeds in applying the principles of physics to bound systems. It is worthwhile emphasizing that we believe that the governing principles of bound systems (as opposed to those of unbound systems) provide the appropriate framework for understanding cold fusion and that this fact has been largely ignored.

The applicable rules of physics for ground state bound systems are that 1) the overlap and other system properties are fully contained in the system wave function that minimizes total system energy, 2) the wave function is constrained by the natural boundary conditions of the environment, and 3) the rules of boson or fermion exchange symmetry (or anti-symmetry) that have been found to apply differently to sets of distinguishable and non-distinguishable particles must be included in an appropriate manner. These principles underlie the physics of atoms and molecules. They are the basis of atomic physics and quantum chemistry. The energy-minimizing wave functions have particle-particle avoidance terms, called correlation terms, which can be, but need not be required to restrict a specific particle A from being present at a point in space when particle B is present. In bound systems near room temperatures the amplitude of these particle-particle avoidance terms is determined by the energy minimization process. An important point is that in bound systems, system energy is constrained to be finite. For this reason, energy minimization principles always apply (often with unexpected results), and can be used to determine the ground state and lowest excited states. In unbound systems, such as plasma, the energy is not constrained to be finite. In this case the use of scattering theory and the associated quantum mechanics is the more appropriate approach for determining system dynamics.

The Helium Atom as an Example of a Bound Physical System
A good example of the physics of bound systems is provided by the calculation of the 2-body wave function that describes the 2 electrons of the ground state helium
atom.\(^2\) The Schrödinger equation for the helium atom (simplified by taking the nuclear mass as infinite) is

\[-\frac{\hbar^2}{2m_e} [\nabla_1^2 + \nabla_2^2] \Phi_s(\mathbf{r}_1, \mathbf{r}_2) + \left[ \frac{e^2}{r_{12}} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} \right] \Phi_s(\mathbf{r}_1, \mathbf{r}_2) = E \Phi_s(\mathbf{r}_1, \mathbf{r}_2)\]

where \(E\) is the band state energy of the 2-electron spatial wave function \(\Phi_s(\mathbf{r}_1, \mathbf{r}_2)\) for the zero-spin state, and \(r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|\). \(\Phi_s(\mathbf{r}_1, \mathbf{r}_2) = \Phi(\mathbf{r}_1) \Phi(\mathbf{r}_2)\) is symmetric with respect to interchange of \(\mathbf{r}_1\) and \(\mathbf{r}_2\). In this equation the \(-\frac{\hbar^2}{2m_e} [\nabla_1^2 + \nabla_2^2]\) term represents the kinetic energy of the electrons, and the \[\frac{e^2}{r_{12}} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2}\] term represents the potential energy. The \(\frac{e^2}{r_{12}}\) term is the 2-electron coulomb repulsion term which results in correlated avoidance behavior by the two electrons.

The variational method was used by Hylleraas\(^3\) to determine a sequence of 2-electron wave functions of increasingly better accuracy. Making use of the elliptical symmetry of the problem he reduced the six independent configurational coordinates of the 2 electrons that appear in the Schrödinger equation, namely \(\mathbf{r}_1\) and \(\mathbf{r}_2\), to three independent elliptic coordinate variables \(s, t, u\) derived therefrom. He also made use of the symmetric spatial exchange symmetry of indistinguishable fermions with anti-parallel spins, which requires that candidate solutions be even functions of variable \(t\). His third approximation is

\[
\Phi_s = e^{-1.82 s/b} \left[ 1 + 0.29 u/b + 0.13 t^2/b^2 \right]
\]

where

\[
s = |\mathbf{r}_1| + |\mathbf{r}_2|,
\]

\[
t = |\mathbf{r}_1| - |\mathbf{r}_2|,
\]

\[
u = r_{12} = |\mathbf{r}_1 - \mathbf{r}_2| = (|\mathbf{r}_1|^2 + |\mathbf{r}_2|^2 - 2 |\mathbf{r}_1||\mathbf{r}_2| \cos \theta)^{1/2}, \text{ and}
\]

\[
b = \text{Bohr radius of hydrogen} = 0.53 \, \text{Å}
\]

Consider what the Hylleraas solution tells us about particle-particle overlap in bound particle systems. The Hylleraas solution is dominated by the exponential decrease in \(|\Phi_s|\) with the mean distance of the 2 electrons from the nucleus, i.e., with \(s/2\). To explore the electron-electron avoidance behavior we study the Hylleraas 6th approximation solution\(^3\) on the surface of a sphere of fixed radius, i.e. \(s\) is fixed and \(t=0\). A plot of the variation of the amplitude of \(\Phi_s\) with respect to the central angle \(\theta\) between the 2 electrons as viewed from the nucleus is given in Fig. 1. The wave function amplitude goes through a minimum at \(\theta=0\), which corresponds to the point \(r_{12}=0\). The wave function amplitude has been normalized to its value at \(\theta=180^\circ\), which corresponds to the 2 electrons being on opposite sides of the nucleus.
Since the wave function amplitude at these two points is not much different, the figure shows that the 2 electrons of the helium atom have substantial overlap; in other words, if the electrons had the fusion capability of deuterons, they would fuse.

![Wave function graph](image)

**Fig. 1** Amplitude of helium ground state 2-electron wave function on the surfaces of 2 spheres for which $s = \text{constant}$. Values have been normalized with respect to the peak values, which occur when the 2 electrons are on opposite sides of the nucleus. Nature uses a cusp at $r_{12} = 0$ to compensate for the infinite electrostatic potential existing at this condition. The values at $\theta = 0$ measure the degree of electron-electron overlap. If the electrons had the nuclear properties of deuterons, they would fuse.

**Wave Equation Singular Points**

The behavior of the 2 electrons of the helium atom is an illustration of the more general behavior of particles in bound systems. The more general Schrödinger equation for electrostatically interacting particles in an external potential $V_{\text{ext}}$ is

$$[-\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_\mathclap{i,j} \frac{e^2}{r_{ij}} + V_{\text{ext}}] \Phi_s(r_1, r_2, \ldots r_N) = E \Phi_s(r_1, r_2, \ldots r_N)$$

where $r_{ij} = |r_i - r_j|$.

The $e^2/r_{ij}$ terms in the wave equation go to $\infty$ at $r_{ij} = 0$. However, because the system is bound, the eigenvalue $E$ is always finite (and less than zero). This means that both the right and left sides of the equation must remain finite. (For unbound systems, $E$ need not remain finite.) This means that at $r_{ij} = 0$, because $e^2/r_{ij} \to \infty$ either $\Phi_s(r_1, r_2, \ldots r_N) = 0$ or $\sum_i \nabla_i^2 \Phi_s = \infty$. In the latter case $\Phi_s(r_1, r_2, \ldots r_N)$ has a discontinuous derivative at $r_{ij} = 0$, i.e. the wave function has a cusp at $r_{ij} = 0$. In
practice Nature (i.e. energy minimization) makes use of both possibilities. If the kinetic energy terms $-\hbar^2/2m \sum \nabla_i^2 \Phi_\text{sc}(r_{ij})$ dominate the energy balance, Nature uses cusp solutions; if the potential energy terms dominate, Nature zeroes the wave function at $r_{ij} = 0$. However, the situation for nuclei in molecules is different than for electrons in the helium atom. For nuclei in deuterated molecules $m$ is the deuteron mass $m_D$, instead of the electron mass $m_e$ used in the He solution. This reduces the importance of the kinetic energy terms by a factor of 3600. This reduction makes the potential energy term dominant. Nature then zeroes the wave function and no fusion is possible. (This condition also applies to any possible interstitial $D_2$ configuration.)

Since interstitial occupations of a metal lattice by $D_2$ are unable to fuse, the cold fusion heat observations require that the $D$ be in some other configuration. We now show that when $D^+$ is in a delocalized configuration, such as a Bloch state, then overlap can occur and fusion becomes possible. 4

**Bound State Systems Containing Band State Ions**

The physics of bound solid state systems depends on the same laws as the physics of molecules. If one considers a Bloch state $D^+$ population in a microscopic crystal resembling an atom cluster, no $D^+-D^+$ overlap can occur because the potential energy coulomb repulsion term in the wave equation dominates the kinetic energy term in determining the magnitude of the correlation terms in the wave function, just as it does in normal $D_2$ molecules. On the other hand, Bloch states have the important property that their amplitudes are periodic functions of the underlying lattice. This means that in a periodically ordered lattice, if the band state $D^+$ ions are spread out over successively larger crystal sizes, i.e. if $N_{\text{cell}}$ is increased, the amplitude of each single particle wave function decreases, and the importance of the wave equation coulomb repulsion potential terms decreases relative to the importance of the kinetic energy terms. As shown below, this behavior means that wave function overlap occurs and fusion becomes possible.

To pursue our argument let us first look at the potential energy reduction that occurs as a result of introducing nodes or cusps into the wave function in order to reduce the amplitude of the wave function when $r_{ij} = 0$. The particle-particle avoidance interaction reduces system potential energy by $\Delta E_{\text{pot}}$

$$\Delta E_{\text{pot}} = 1/2 \int \int e^2 I \Phi_{\text{corr}}(\mathbf{r})^2 I \Phi_{\text{corr}}(\mathbf{r'})^2 I d\mathbf{r} d\mathbf{r'}$$

$$- \frac{1}{2} \int \int e^2 I \Phi(\mathbf{r})^2 I \Phi(\mathbf{r'})^2 I d\mathbf{r} d\mathbf{r'}$$

where within the many-body wave function

$\Phi$ is a single particle Bloch function without correlation terms, and

$\Phi_{\text{corr}}$ is a correlated single particle function that also possesses Bloch function symmetry but is derived with $r_{ij}$ avoidance terms (which results in dimples: nodes or cusps).
The particle-particle avoidance increases system kinetic energy by $\Delta E_{ke}$

$$\Delta E_{ke} = \hbar^2/2m_D \int \nabla \Phi^* \nabla \Phi_{corr} \, dr - \hbar^2/2m_D \int \nabla \Phi^* \nabla \Phi \, dr$$

where

$\nabla \Phi$ is the gradient of the wave function without correlation terms, and

$\nabla \Phi_{corr}$ is the gradient of the correlated wave function with $r_{ij}$ avoidance terms (nodes or cusps).

With increasing $N_{cell}$ both $1 \Phi 1^2$ and $1 \nabla \Phi 1^2$ decrease as $1/N_{cell}$. Since on a per unit cell basis $\Delta E_{pot} \propto 1 \Phi 1^4$, $\Delta E_{pot}$ decreases as $1/N_{cell}^2$. In contrast, $\Delta E_{ke} \propto 1 \Phi 1^2$. Then, at large $N_{cell}$ it follows that $\Delta E_{ke}$ dominates $\Delta E_{pot}$. This resulting dominance of kinetic energy over potential energy in the part of the wave equation controlling particle-particle avoidance means that total energy is minimized in a similar manner to the way kinetic energy dominance leads to energy minimization and overlap of the electrons of the ground state helium atom. As a result the many-particle energy-minimizing wave function has only a small amount of correlation wave function curvature, and has a shallow cusp at $r_{ij}=0$, i.e. particle-particle overlap is almost complete.

As discussed in the next paragraph $D^+$ ion band state fusion energy is released in a distributed fashion. The comparison between the $D^+$ ion band state picture including nuclear energy release and the situation involving the balance between kinetic energy and coulomb repulsion between electrons in the helium atom is especially meaningful provided the distributed nuclear energy release per unit cell is of the order of the characteristic $D^+$ vibration energies, which are in the 0.01 to 0.1 eV range. Since the distributed nuclear energy release = 23.8 MeV/N_{cell}, this requirement is that $N_{cell} > 10^8$. Since the kinetic energy term in the wave equation relative to the potential energy term is reduced by the order of $10^4$ in going from the electrons in the helium atom to $D$ in the $D_2$ molecule, the value $N_{cell} = 10^8$ is much greater than that needed to meet the requirement for $D^+-D^+$ overlap. Thus with $N_{cell} = 10^8$, the essential overlap requirement for $D^+-D^+$ fusion is satisfied.

**Why Ion Band State Fusion Is Radiationless**

We now consider why $D^+$ ion band state fusion produces no $\gamma$-rays or energetic particles. Interaction between band state occupations makes only a small amount of nuclear energy available in each unit cell. This is because, when both the reactants and products of the potential nuclear reaction occupy band states, only a small fraction of each reactant and product is located in each unit cell, meaning that only a small amount of each reaction occurs in each unit cell. In contrast, high energy particle and $\gamma$-ray emission requires concentration of the available energy into a small volume. At the near room temperature conditions used in cold fusion studies concentration of the available energy into a single unit cell by incoherent or
coherent processes is statistically impossible because of the large entropy cost associated with accomplishing this process.

**Where the Energy Goes**
The small amounts of energy made available in each unit cell by the $2D^+_{\text{band}} \rightarrow ^4\text{He}^{++}_{\text{band}}$ reaction should be able to excite phonons, either thermally (through residual electron-ion interaction), or at the boundaries of the lattice where periodic order is lost. The large density of states that is provided by these processes is responsible for making the nuclear reactions irreversible. At low temperature, phonon generation occurs primarily at the boundaries of the crystal lattice, where periodic order is lost. In these regions, the electron-ion interaction is dominated by the requirement that the "spill-out" dipole layer associated with electrons near the surface and the surface ion band states adjust themselves in a manner that is consistent with Gauss's law and the applied electric field. (In the surface region, as opposed to the bulk, it is possible for a net distribution of charge to be present because there exists a net electric field flux into and out of this region.)

Although this readjustment process is dominated by the behavior of the electrons and the associated electron-ion interaction, it is possible to identify a prospective ground state ion configuration in the surface region that is consistent with the arrangement of electrons. In particular, at the surface, although three dimensional periodic order is lost, at low temperature, it is plausible (depending on loading conditions) that two dimensional order (defined by the lattice structure in planes parallel to the surface) will be present. Then, the same kinds of ion band state (as well as electron band state) considerations apply except that Bloch symmetry in this case applies only in directions parallel to the surface. In directions normal to the surface, each wave function is smoothly matched onto the appropriate solutions of the Schroedinger equation. The result of this construction is that each bulk-like (electron or ion) band state smoothly matches onto a surface state which possesses two-dimensional Bloch symmetry in the surface region (where the net electric field flux is non-vanishing), and exponentially decays in directions normal to the surface, in a manner similar to the exponential decays that occur in all negative kinetic energy region solutions associated with the bound state Schroedinger equation.

In the extreme low temperature limit it is plausible that the dominant phonons will result from extreme long wavelength acoustical phonons in which large portions of the bulk lattice effectively resonate with respect to each other. This is because these phonons, which can be generated through small fluctuations in the electrostatic zero (by the average value of the chemical potential), 1) are the most sensitive to the smallest variations in charge in the surface region, and 2) can also result from the large density of states associated with intermediate "horizontal" (or UmKlapp) processes, in which the lattice (or a large portion of the lattice) effectively recoils as a whole. An additional possibility is that long wavelength optical phonons will be generated through the volumetric stress associated with each fusion. Although it might appear that the possible modes of energy release associated with these optical phonon processes would occur with higher energies (and temperatures) than the
ones associated with long wavelength acoustical phonons, each fusion includes an
effective softening of the ion band state in the zero-point motion of the ion band
state material (owing to the larger mass of the $^4$He$^{++}$ product).

**Ion Band State Matter as a Matter Field within a Host Lattice**

Limitations on cold fusion possibilities are determined in major part by limitations
on allowed final state wave functions. To the extent that the coulomb barrier terms
in the many-body wave function have vanishing amplitude, the ion band state
approximates a non-relativistic quantized matter field$^5$ restricted to a finite volume
$V_{\text{xtal}}$. For a $D^+$ band state population the quantum of mass is 2 AMU, i.e. the matter
content of the field can only increase or decrease in discrete steps of 2 AMU. Within
the matter field there is concurrent action at a distance, as required to resolve the
Einstein, Podolsky, and Rosen$^6$ argument against the completeness of quantum
mechanics. An important point is that the ion band state picture only makes sense
if the ion bands remain occupied for a sufficiently long period of time relative to the
required time necessary for nuclear reaction to proceed. For this to occur, each
nucleus that occupies such a state must effectively dissociate from its own electron
(as well as the remaining electrons) over a time scale that is short with respect to
times associated with electrostatic processes, but long relative to nuclear process
time scales. This requirement places important constraints associated with the
underlying electronic structure on the kinds of environments where ion band state
matter will form in a manner that will allow for appreciable nuclear reaction to
occur.

The physical system includes the crystal interior lattice, the crystal surface boundary
region where periodic order is lost, the interior $D^+$ ion band state matter field, and
the matter field's surface stress region within which the band state matter wave
function transitions into a decaying exponential, associated with the negative
kinetic energy region outside the solid. The final state consists of bulk-like ion band
state $^4$He$^{++}$, which depending on the temperature and degree of crystalline order in
the surface region, may match onto any of a variety of functional forms in the
surface region. In the extreme low temperature limit, as mentioned above, the ion
band states can match onto localized surface states provided adequate crystalline
order is present in planes parallel to the surface. An interesting point about this case
is that these ion band surface states in principle can couple coherently to electron
surface states (occupied by the host electrons as well as by the injected electrons that
accompany the ion band state $D^+$) in a manner that could preserve Bloch symmetry
in planes parallel to the surface. The significance of this form of coupling is that
neutral or ionized $^4$He could be ejected from the solid in a coherent manner,
leading to a Bragg-like diffraction pattern, reminiscent of the diffraction patterns
that are observed in low-energy $^4$He scattering experiments. In all cases, the large
strain energies (and propensity for cracking, etc.) associated with multiple
occupation of a unit cell by either D or He in a non-ion-band-like form, inhibit the
final state $^4$He$^{++}$ from occupying or coupling to non-ion-band-state $^4$He in bulk
regions. This is the justification for the prediction that we made$^4,7$ prior to the
experimental measurements\textsuperscript{8,9} that the $^4\text{He}$ product should be found primarily at low energy and in regions outside heat-producing electrodes.

**The Reaction Process**

In the above picture there is no intermediate observable state between ejection of a normal $^4\text{He}^{++}$ product and annihilation of 2 deuterons in the matter field. The normal astrophysical factors affecting fusion rate apply. The $D^+ - D^+ \rightarrow ^4\text{He}^{++}$ reaction would be restricted only by the requirement for anti-parallel spins, which, in most cases, reduces the reaction rate by a factor of 3. This last reduction factor would be reduced in a situation in which band state $D^+$ is preferentially prepared so that spin populations of opposite spin are equally occupied. An interesting point is that by introducing a constant magnetic field $H$ (or a constant magnetic field $H$ accompanied by a perpendicular oscillating magnetic field, as in standard NMR measurements), it is possible to enhance both 1) spin allignment in directions parallel to $H$ and 2) anti-allignment of spins in directions perpendicular to the field. It is also interesting to note that the creation of $^4\text{He}^{++}$ in ion band state form provides a source for reducing magnetism (since $^4\text{He}^{++}$ is non-magnetic while the feedstock ion band state $D^+$ is magnetic) in a delocalized manner that preserves periodic order. We have also shown\textsuperscript{4,10} that for low $^4\text{He}^{++}$ concentrations, the fusion rate is proportional to the concentration of final state $^4\text{He}^{++}$. As discussed below, it also is true that reductions in periodic order inhibit fusion. Together these observations suggest that the process of creating $^4\text{He}^{++}$, which is enhanced by preferentially preparing the feedstock $D^+$ in a form in which equal populations of anti-parallel states are occupied, may help to preserve both crystalline and magnetic order in a manner that may further enhance the fusion process.

As discussed in part 2, the above picture conforms to the requirement of Born-Oppenheimer separability of the fast nuclear reactions with respect to the slower electrostatic interactions that affect only the center-of-mass coordinates. The nuclear/zero-point-motion volume ratio $V_{\text{nuc}}/V_{\text{zp}}$ enters in as described in our 1991 *Fusion Technology* paper\textsuperscript{4}. In contrast, reactions of the type $H^+-H^+$ going to a deuteron by electron capture or positron emission with emission of a neutrino would probably be excessively slow due to the required weak force interaction.

2. $D^+$ Ion Band State Fusion

**Exotic Situation, Not Exotic Physics**

The arguments presented above show that cold fusion is not the result of exotic physics; instead it is mainstream physics applied to an exotic situation that can only occur inside condensed matter. It is the result of the formation of exotic types of compounds, wave-like occupations of energy bands, which become allowable when chemical thermodynamic conditions support their formation. We have suggested several types of compounds that could include such ion band state occupations, namely, $\text{PdD}_1$, $\text{AgD}_6$, or $\text{NiD}_6$. However, the designation $\text{PdD}_1$ should not be taken too literally. Although it describes conditions that might allow ion band state
formation at low temperature, some $D^+$ ion band state occupation will occur in $\text{PdD}_x$ with $x<1$ even at low temperature. The cause of such occupations is the entropy term in the chemical potential associated with occupation of a fixed number of interstitial sites.\textsuperscript{11} This term forces the chemical potential for D absorption to become infinitely positive before the value $x=1$ is reached. Equally important, at finite temperature, some occupation of the band state would occur at $x<1$ even if the entropy term were not included. (Band state occupations are only required to occur over some finite lifetime that is considerably shorter than the typical time-scales associated with the dominant thermodynamic processes. Band state occupations occur only over a finite volume $V_{\text{xtal}}$, where $V_{\text{xtal}}$ can be a sub-volume of the entire crystal.) The temperature dependence of excess heat production reported by Storms\textsuperscript{12} suggests an energy of activation of ~15 kcal/mol for populating the heat release state, which we assume to be the band state. The proper designation for the palladium deuteride that supports fusion is $\text{PdD}_1\cdot\eta+\delta$, where $\eta(T) << 1$.

The exotic character of the $D^+$ band state matter state is shown in part by the very small concentration of ions required for the production of measurable heat. Calculations indicate that an occupation density of $\sim10^{-7}$ band state $D^+/\text{unit cell}$ is sufficient to explain observed heating rates. Moreover, there are limitations on the top end values of $x$ that are compatible with heat production. A population of $\delta >10^{-3}$ may be sufficient to force occupation of the Pd tetrahedral interstitial sites in $\text{PdD}_x$, which may destroy the periodic order needed for power production. The range in values of $x$ that correspond to these $\delta$ limits may be quite restricted. The drop in resistivity observed by McKubre\textsuperscript{13} in $\text{PdD}_x$ once $x$ exceeds ~0.73 is a qualitative measure of lattice order. Only the portion of D absorbed into Pd that increases ordering is important to the band state fusion process. Hydrogen uptake measurement of $x$ can sometimes be misleading since other non-productive means of containment of D exist, e.g. filling of interstices, occupations of tetrahedral sites in octahedrally loaded metal, and possibly some kind of LiD,Pd alloying. Another important factor affecting ion band state formation in the different metals is host electronic structure.

**Experimental Evidence for the Existence of Band State Hydrogen**

Although $D^+$ ion band state matter may be considered exotic, 2-dimensional ion band state matter is known to be present in H and D adsorptions on the surfaces of transition metals. This idea has been used to explain the vibrational spectra dependence on H- and D- coverage in the adsorptions of H and D on Cu(110) and Ni(100).\textsuperscript{14,15} Ion Band State occupation potentially can be used to explain the huge diffusion lengths of D and H in many metals.

**Role of Electronic Structure**

An important aspect of ion band state occupation and the implications of ion band state occupation to cold fusion, that we have not emphasized in the past, is the role of electronic structure. Normal chemistry at room temperature inherently favors neutrality (or approximate neutrality). It is well known that this is true in the solid
state and this fact has been the cornerstone for understanding a large number of the cohesive, chemical, and electronic properties of solids. For this reason D+ ion band states can become occupied and ion band state mediated fusion can occur only if specific conditions associated with the underlying electronic structure are fulfilled. 1) Sufficient periodic order must be present for a sufficiently long period of time. 2) Deuterium and host electrons must dissociate from D+ band-state matter on timescales that are long compared with those required for fusion through nuclear self-interaction. 3) D+ band-state matter must distribute itself in a sufficiently diffuse manner as a result of interactions with the host lattice.

In the case of Pd and PdD, we know from neutron diffraction experiments\textsuperscript{16} the structure of PdD, the presence of crystalline order, the location of the D, and its characteristic zero-point motion radius, which is relatively large (~0.2\text{\AA}). We know from the excellent agreement between a number of first-principles ab initio electronic structure calculations\textsuperscript{17} and photoemission experiments\textsuperscript{18} even some of the more delicate aspects of the associated electronic structure of both Pd and PdD, to a fair level of precision. Thermodynamic modeling\textsuperscript{11}, and electronic structure calculations in particular, show that in PdD\textsubscript{x} as x is increased from values below 0.7 to unity, chemical bonding involves important hybridization between bonding 4d states and anti-bonding 5s states provided by the Pd.

In the case of the PdD\textsubscript{1-\delta} that we have suggested is relevant to cold fusion, within the bulk, in each unit cell the concentration (\text{\delta}) of ion band state D+ is balanced by an equal concentration of electrons (which also occupy band states). The assumptions that both the D+ and the electrons may fractionally occupy band states in this manner is not only consistent with the known laws of solid state physics, it is consistent both with thermodynamics\textsuperscript{11} and with the electronic structure calculations\textsuperscript{17}. In particular, Wicke and Brodowsky\textsuperscript{11} have summarized the behavior of the chemical potential with respect to changes in D-loading. Their figure 3.11 shows that large lattice strain energy costs are associated with D-occupation of a Pd unit cell when x is small, from which one concludes that huge lattice strain energy costs would be associated with D-occupation of a unit cell by more than one D in the limit that x\rightarrow1+\text{\delta} in PdD\textsubscript{x}. This result essentially is tied to the dominant Pd-to-H bonding-anti-bonding features associated with the 4d-5s hybridization identified by Papconstantopoulos el al.\textsuperscript{17}.

An important point is that it follows from a minor generalization of local density theory\textsuperscript{19} (which provides the basis of these calculations) that, when \delta is sufficiently small, as D is loaded into PdD to form PdD\textsubscript{1-\delta}, the energy associated with the accompanying additional concentration (\delta) of electrons is minimized provided 1) these electrons fractionally occupy the lowest unoccupied states (immediately above the PdD Fermi level), and 2) variations in electronic structure associated with these fractional occupations does not alter the density of ion band state deuterons. Although it is not rigorously necessary to impose these last two constraints, it does follow rigorously that they provide a means of constructing a self-consistent local
density approximation method for determining the ion band states in the limit in which $\delta$ becomes infinitesimally small. This minimization of electronic energy requires that the added $D^+$ be in a band state.

Additional results of Papaconstantopoulos et al. suggest that variations in electronic structure associated with fractionally occupying new states immediately above the Fermi energy $E_F$ of PdD probably would not appreciably affect the ion band state densities that we have used previously, nor would the densities differ importantly from those that would result from self-consistent local density approximation calculations carried out in this fashion. These earlier ion band state calculations were carried out using minimum uncertainty wave packets of a characteristic size defined by the known zero-point motion volume of D in PdD. Papaconstantopoulos et al. have shown that, as a result of the 4s-5d hybridization discussed above, near $E_F$ electron occupation involves anti-bonding 5s-like states primarily in regions in the vicinity of Pd ion cores, and only a very small (-0.1 e), predominantly s-like electronic charge is found in the vicinity of the octahedral site zero-point-motion volume in which deuteron cores are known to bind to the solid.

Both results indicate that effectively $D^+$ ions do dissociate from host electrons on time-scales that are large enough to allow for fusion to occur. In particular, in ref. 21, we have used the minimum uncertainty packets mentioned above to determine meaningful bounds on the electrostatic ion-ion self-interaction, which we find to be $\sim 10^{-17}$ second. This value, which is the rate-limiting effect associated with the coulomb repulsion between potentially interacting $D^+$, is much smaller than the time-scales ($\sim 10^{-14}$ s) associated with the 10's of meV bandwidths characteristic of the coupling between $D^+$ and electrons in PdD. This value is also considerably larger than the typical time-scales ($\sim 10^{-22}$ s) associated with nuclear self-interaction.

It is worthwhile noting in passing that it is possible to consider generalizations of the above picture associated with relaxing the restriction (implied by local density theory) requiring that variations in ion band state density become independent of variations in electron band state density. This restriction applies rigorously for the ground state wave functions provided electron-ion-band-state correlation effects are not present that could lower system energy. Although in the extreme low ion concentration limit, these correlation effects must become unimportant, it is possible that, at finite ion band state concentrations, electron-ion pairing mechanisms could lower system energy in a manner similar to the way pairing between electrons through phonon coupling to the lattice lowers system energy in the formation of Cooper pairs. Waber has identified this possibility and suggested potential nesting features in the Fermi surface associated with the fractionally occupied electronic states that could trigger these forms of correlation.

**Transistor vs Vacuum Tube Thinking**

To visualize the cold fusion process one must adopt a different mode of thinking relative to that employed in hot fusion and conventional nuclear physics. In hot fusion one thinks in terms of collisions between randomly moving ions. These
collisions are analogous to the electron-electron collisions that electrons undergo in the electron cloud surrounding the hot filament of a vacuum tube. To visualize the cold fusion process one must switch from thinking about the localized discrete particles encountered in "vacuum tube thinking" to thinking in terms of the collective action of the delocalized wave-like "particles" existing in semiconductors, i.e. to "transistor thinking". Once an individual D occupies an ion band state, it no longer is located in any specific unit cell. It is located everywhere. This is analogous to the behavior of electrons in metals. Potential interactions and modes of interaction are altered dramatically. More importantly, the coulomb barrier idea of particle-particle Gamow theory is replaced by the correlation properties of the many-body wave function.

**How Ion Band State Nuclear Reactions Occur**

The physics of collectively interacting wave-like ions has substantial implications with respect to potential nuclear interactions. Under the rules of solid state physics, cold fusion can occur as a transformation of wavelike deuterium into wavelike $^4$He. As previously discussed$^4,^7,^10$, the energy release from the transformation involves no high energy concentration, and no high energy particles are emitted. The nuclear interactions are governed by a self-consistent, non-relativistic quantum field theory that we have named Lattice Induced Nuclear Chemistry (LINC)$^7$. LINC is based on ordinary non-relativistic quantum field theory as it should apply to an indistinguishable collection of ion band state D (also called a Bose Bloch condensate) corresponding to the small band state concentrations $\delta$ of D+ associated with the PdD$_{1+\delta}$, AgD$_{\delta}$, and NiD$_{\delta}$ compounds. Energy is minimized through elimination of lattice stress and by the occupation of uncorrelated many-body wave functions that are constructed from single particle ion band states. The resulting potential nuclear reactions preserve the requirement that the locations of both the potentially reactive D and the reaction products cannot be determined on the time-scales associated with maintaining periodic order.

**Born-Oppenheimer Separability and Selection Rules of LINC**

Through LINC, transistor-like (i.e., distributed solid-state-like) as opposed to vacuum tube-like (collision dominated) rules about particle overlap and transport become valid. The mathematical basis for this is provided by the underlying assumption of LINC and its reactions: reactions and overlap can occur provided the dominant electrostatic interactions are between the lattice and the center of mass of potentially nuclear reactive nucleons, and not between the individual nucleons. This limit can occur when amplitudes of the ion-ion correlation terms in the many-body wave function become small, and provided the time-scales for nuclear reaction are very much shorter than those associated with electrostatic interaction.

When the time-scales for particular nuclear processes are very different than those associated with the motion of the nucleus within an applied electrostatic field, it then becomes appropriate to write the wave function of the nucleus as the product of a rapidly varying function that describes the motions of the individual nucleons.
within the nucleus relative to the center of mass \( r_{cm} \) multiplied by a more slowly varying function that describes the center of mass motion of the nucleus with respect to the applied electrostatic potential. This factorizing of the wave function is referred to as Born-Oppenheimer separability. This assumption holds rigorously provided the time-scales associated with the center of mass motion and the motions of the individual nuclei always remain very different. This representation applies to the initial state provided the center of mass motion of each \( D^+ \) is well-described by a band state. Expressed in terms of the separation coordinates of the protons and neutrons in p-n pairs \((r_n-r_p)\), the wave function of each deuteron is given by

\[
\Phi(r_n, r_p) = \Psi_{nuc}(r_n-r_p) \Psi_{band}(r_{cm})
\]

where \( \Psi_{nuc} \) is the rapidly varying nuclear wave function that describes the probability amplitude of finding a proton or neutron within a small volume centered about the center of mass, and \( r_n \) and \( r_p \) respectively are the locations of the proton and neutron.

The assumption of LINC is that this form of Born Oppenheimer separability applies rigorously as a function of time in all multi-particle fluctuations (governed by the underlying field theory) that are consistent with the requirements that the nuclear and electrostatic time scales associated with these fluctuations remain very different. This means that at any time during the reaction the final state must be representable in a Born-Oppenheimer separable form:

\[
\Phi(r_1, ..., r_m) = \Psi_{nuc}(r_1-r_{cm}, ..., r_m-r_{cm}) \Psi_{band}(r_{cm})
\]

where \( \Psi_{nuc}(r_1-r_{cm}, ..., r_m-r_{cm}) \) now describes the nuclear (multiple-nucleon) wave function. In refs. 7 and 10, we have derived important selection rules associated with this constraint. In particular, the constraint automatically rules out a large number of potential reactions. This is because the constraint is only meaningful provided 1) zero-point motions of the center of mass of potentially reacting nuclei are sufficiently large both during and subsequent to the reactions, and 2) these center of mass motions must remain independent from the motions of the individual nucleons at all times during the reaction.

Because nuclear reactions between closely separated nucleons are always independent of the absolute location of the center-of-mass, there exists an important symmetry which insures that the final state representation is meaningful since it preserves this symmetry. Because of the requirement that the zero-point motions of the center of mass must be sufficiently large, the limitations of the representation are closely tied to the underlying electronic structure. Using reasonable wave functions, based on known values of zero-point motion for \( D \) in \( \text{PdD}_x \), we have estimated in refs. 7 and 20 suitable bounds for the electrostatic self-interaction and

10-15
nuclear self-interaction, where we have shown that separability can be expected to apply for a $^4$He product.

Perhaps of greater significance is the following: The assumption that Born-Oppenheimer separability must be maintained in the final state and during all intermediate states involving multi-particle fluctuations associated with band state overlap leads to an important selection rule. Beginning from a state consisting entirely of $D^+$ ion band states, the many-nucleon portion of the final state wave function $\Psi_{\text{nuc}}(r_1, r_{\text{cm}}, \ldots, r_m, r_{\text{cm}})$ must be formed exclusively from unbroken proton-neutron pairs.

As we have shown in ref. 10, this rule is based on rigorous requirements associated with constraining the governing field theory so that the nuclear and band state wave functions evolve independently from each other. We have demonstrated this using the defining constraints of canonical quantization (using Poisson Brackets) associated with the problem of constructing a field theory that maintains Born-Oppenheimer separability starting from an initial state consisting of ion band state $D$. We have previously used the terminology $^{7,20}$ "bosons in and bosons out" to refer to the resulting selection rule that proton-neutron pairs cannot be broken.

The presence of unpaired proton-neutron pairs, or of unpaired protons or neutrons, in the initial state requires that this rule be modified. In ref. 10, we have discussed these modifications. The resulting selection rules and reactions associated with LINC, both when either unpaired protons and neutrons are and are not present, are summarized below.

**Many-body Wave Function**

The initial state many-body wave function is constructed from a summation of terms. Each term consists of a product of all of the single deuteron wave functions in which each deuteron is assigned a specific location. The summation imposes the required particle-exchange symmetry, ensuring that the many-body wave function describes indistinguishable bosons. Because of Born Oppenheimer separability, automatically, the summation of terms can be factored into a product consisting of a single factor derived from a subproduct of the localized wave functions ($\Psi_{\text{nuc}}$) multiplied by a sum of terms associated with the slowly-varying band state $D^+$ many-body function. (Because of Born Oppenheimer separability, the effects of particle exchange symmetry of the entire many-body function appear only through the many-body band state wave function.) Band state $D^+$ matter has magical properties that are implicit because of the exchange symmetry that is embodied in the many-body band state wave function. Because each single particle band state wave function has Bloch function symmetry, when the many-body band state wave function becomes occupied, the lattice strain (associated with injection of non-band state $D$ into the host) vanishes. For this reason, this function minimizes system energy in crystals that are sufficiently large, when the number of band-state $D^+$ is
much less than the total number of unit cells, and the band state $D^+$ remain uncorrelated.

This many-body wave function can also be written in a "vacuum tube-like" form, based on a particle-like (Wannier state) representation\textsuperscript{4}. The resulting description is characterized in a manner involving particle-like occupations (involving whole numbers of $D^+$), in which each occupation is transient and possesses a finite life time $\Delta t$. Specifically, $\Delta E \Delta t = h$, $\Delta t = 10^{-16}$ s. The particle-aspect of the matter field's behavior is shown in the Wannier form (analogous to an inverse Fourier transform) of the many-body bosonic wave function\textsuperscript{4}.

$$\Psi(P, r) = \frac{1}{ND} \frac{1}{2} \sum (1/N_{\text{cell}})^{NB/2} \left\{ \prod \sum \Phi_s(r_m) \exp(i k_p \cdot R_s) \right\}$$

Here $(r_m)$ means the sum is over all products in which distinct pairs of particles are exchanged. All terms are of the form

$$\Phi_{121}(r_{11}) \Phi_{61}(r_{77}) \Phi_{18214}(r_{480}) \Phi_{2107}(r_{396}) \cdots \cdots \Phi_{97}(r_{11}) \cdots$$

Each term contains $N_D$ factors, where $N_D$ is the number of deuterons in the many-body band state. There are $N_D! (N_{\text{cell}})^{N_D}$ terms in the wave function. In the many-body wave function the deuteron index never repeats, but the unit cell index may repeat. The expansion contains terms that correspond to zero, single, double, triple, etc. occupations of specific unit cells. The existence of multiple occupation terms reveals that $D^+ - D^+$, or $D^+ - D^+ - D^+$, etc. overlap can occur. In other words, the algebraic properties of the many-body wave function imply that overlap occurs. The underlying reason that this becomes possible is that in the localized, Wannier representation, occupation of an individual site can become short-lived. Another way of understanding this point is that in the "usual" (or vacuum tube) way of looking at deuterons, they appear to be long-lived particles, while if a collection of them occupy ion band states, this particle (i.e., Wannier state) picture can breakdown because the lifetime of a "particle" at any individual location can become very short. Underlying the resulting overlap process is this question of lifetime. If the lifetime for electrostatic overlap (as a result of the band state occupation) is considerably longer at a lattice site in this "particle-like" representation than the comparable "particle-like" lifetime associated with nuclear decay, nuclear reaction can occur. As a result, a variety of reactions become possible.

\textbf{The 2-body Reaction}

The number of double occupations of unit cells exceeds the number of triple occupation by the factor $1/\delta$, where $\delta$ is the number of band state ions per unit cell.
Since $\delta$ may be of the order of $10^{-6}$, 2-body interactions are expected to dominate. All the reactions involve delocalized D$^+$ ions and proceed as volume distributed interactions. The first reaction step is a reversible coalescence of p-n pairs

$$2D^+ \rightleftharpoons 4He^{++}.$$ 

The reaction is made irreversible by excitation of the lattice

$$4He^{++} + \text{lattice} \rightarrow 4He^{++} + \text{lattice}^*.$$ 

Helium is ejected from the lattice either as a neutralized surface species

$$4He^{++} \rightarrow 4He^{++}\text{surface}$$

$$4He^{++}\text{surface} + 2e \rightarrow 4He\text{surface}^+$$

or (as discussed above), at low temperature, possibly as a Bragg scattered neutral atom or ion. The species in italics are delocalized configurations (Bloch states). The surface ejection of He was predicted before being observed. In the 2-body reaction overlap of p-n pairs allows nuclear fusion $2D \rightarrow 4He$. (As little as 0.3 ppm of wavelike D$^+$ may be needed to produce 600 W/cc.)

**Multiple- and Mixed-body Reactions**

Other interactions between band states include the three body reactions

$$3D^+ \rightarrow 4He^{++} + D^+$$

and

$$2D^+ + 1H^+ \rightarrow 3H^+ + 1H^+ + 1H^+.$$ 

where the small arrows indicate the relative directions of nuclear spins. The latter reaction requires occupation of both deuteron and protium band states, and has been suggested as a possible tritium-creating band state side reaction. In all the reactions energy release is distributed over the lattice, only a small amount occurs in each unit cell. (As applied to a proposed "normal" water reaction, concentrations of $10^{-7}$ D/Pd and $10^{-3}$ H/Pd may be adequate to produce claimed heat.)

**Predictions**

Predictions made before experimental verification include the requirement for $-1:1$ D/Pd ratio (McKubre et al., Kunimatsu et al.), no appreciable radiation or neutrons (many groups), and primary products being heat and low-energy $^4$He in the outgases (Miles et al., Yamaguchi and Nishioka). Cracking, overloading, and
Other processes that cause loss of periodic order should impede cold fusion heat release.

Other predictions include: Reactions are fractional, involving infinitesimal energy release in each unit cell. Energy is transferred to the lattice through coupling to phonons, excitation of high frequency sound modes, inelastic scattering of products with host electrons, etc. Lattice disintegration terminates heat generation. High energy particle release may occur if periodic order is lost suddenly. Optimal heating occurs when lattice disintegration is minimized, with energy release occurring dominantly through extreme long-wave phonons caused by release of products in regions where periodic order is lost. Reaction products are distributed at surfaces, near cracks, at interfaces, and in the out-gases. At low temperature, lattice termination and motion may induce nuclearly mitigated near-surface stresses, leading to the potential for surface isotopic anomalies (Rolison effect). We interpret these anomalies to be the result of stress imbalance and not a direct nuclear isotope reaction. At sufficiently low temperature, if a single crystal is used, outgassing products (primarily $^4$He) will distribute themselves in the form of a Bragg diffraction pattern. Also, we find $^4$He++ that fusion rate is proportional to the concentration of final state ion band state $^4$He++, suggesting that the reaction possibly has a "self-triggering" mechanism, possibly consistent with a number of run-away heating episodes that seem to have been observed. We also find that steady-state power density should be proportional to current density.

Conclusion
There is experimental evidence for cold fusion which is difficult to explain away. The poor repeatability is understandable in view of the nonequilibrium chemistry required for creating PdD$_{1+6}$ and the problem of cracking due to differential expansion during D loading. There exists a quantum mechanics rationale by which release of fusion energy in a solid can occur without production of energetic particles. This energy release requires the presence of delocalized wavelike D$^+$ and involves a volume distributed reaction.

References