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Conventional physics can explain cold fusion excess heat

S. R. Chubb*

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Abstract

In 1989, when Fleischmann, Pons and Hawkins (FP), claimed they had created room temperature, nuclear fusion in a solid, a firestorm of controversy erupted. Beginning in 1991, the Office of Naval Research began a decade-long study of the FP excess heat effect. This effort documented the fact that the excess heat that FP observed is the result of a form of nuclear fusion that can occur in solids at reduced temperature, dynamically, through a deuteron (d)+d□4He reaction, without high-energy particles or □ rays. A key reason this fact has not been accepted is the lack of a cogent argument, based on fundamental physical ideas, justifying it. In the paper, this question is re-examined, based on a generalization of conventional energy band theory that applies to finite, periodic solids, in which d's are allowed to occupy wave-like, ion band states, similar to the kinds of states that electrons occupy in ordinary metals. Prior to being experimentally observed, the Ion Band State Theory (IBST) of cold fusion predicted a potential d+d□4He reaction, without high energy particles, would explain the excess heat, the 4He would be found in an unexpected place (outside heat-producing electrodes), and high-loading, x□1, in PdDx, would be required.

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1. Introduction

In 1989, when Fleischmann and Pons (FP) [1] made their initial cold fusion announcement, considerable confusion occurred. A key reason for this involved a misunderstanding about what they actually found in their experiments. Initially, everyone believed that Jones *et al*. [2] and Fleischmann, Pons, and Hawkins discovered the same thing: "cold fusion." Jones did observe neutrons, but they probably came from either a very low-level, conventional hot fusion reaction, or some other nuclear

* Corresponding author. Tel.: 703-309-0493; fax: +0-000-000-0000 .
E-mail address: scott.r.chubb@alumni.princeton.edu .

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process that does not involve fusion; while although FP initially claimed they found neutrons, they found them at a level that was a billion times too low to explain their most important discovery: excess heat.

In fact, it is known now that the large amounts of excess heat that FP observed occurred from a form of fusion, but not hot fusion. FP discovered their excess heat from a nuclear reaction that occurs when a deuteron (*d*) fuses with a second *d*, to form ^{4}He, without the "usual" gamma ray that occurs in one of the conventional (but infrequent) hot fusion reactions. Because FP's discovery is fusion, but not hot fusion, the name cold fusion actually fits, and it is more appropriate to think of the neutrons that Jones and FP found as occurring either from hot fusion or through Low Energy Nuclear Reactions (LENR) that do not involve fusion; while the reaction that created excess heat that FP found is cold fusion, and it has no neutrons.

Although considerable controversy followed the initial announcements, research at a small number of laboratories continued. And with time, this number has grown significantly. Even at an early stage in the associated research, the amounts of excess heat that were observed, which were so large that they could not be accounted for by any possible chemical energy process, were confirmed by a number of experienced electrochemists and material scientists. Some of the individuals who were involved in the more important, early successful experiments were McKubre, Tanzella, Crouch-Baker, Huggins, Oriani, Bockris, Miles, and Arata and Zhang, as documented in the book by Beaudette [3].

The Office of Naval Research conducted a decade long study that also documented the heat is real and that it occurs from the $d+d\rightarrow {}^4He$ reaction [4]. The most precise and quantitative relationship between total amount of excess heat that accumulates over time and the comparable accumulation of helium atoms was reported by McKubre *et al.* [5]. Here, it was found necessary to chemically thermally cycle the palladium cathodes to drive much of the helium out of the metal into the gas phase. An important, more recent development is the fact that excess heat can be created through the same kind of d+d$\rightarrow^4$He reaction (without high energy particles) when deuterium gas is loaded into nanometer scale crystals of Pd and other composite materials involving Pd [6].

Talbot Chubb and the author suggested in 1989 that deuterons (d's), in fully-loaded palladium deuteride (PdD), could behave very differently than in free space, by occupying the kinds of states (energy band states) that electrons occupy in periodically ordered solids. Based on this conjecture, it was suggested [7, 8, 9] that the normal rules about fusion might not apply to the cold fusion (CF) claims by Fleischmann and Pons (FP) and that it might be possible to account for what FP suggested through alternative forms of fusion that could result from the very different physical situation that might be possible, as a consequence. Because evidence exists [10, 11, 12] that in certain situations, hydrogen and deuterium nuclei occupy these kinds of "wave-like," ion band states (IBS's) in Casella [13] and on the surfaces [10, 11, 12] of transition metals, a physically plausible argument can be made that the starting point of the associated argument makes sense.

Because d's are bosons, on the length scales associated with conventional electromagnetism, implicit in this hypothesis is the idea that by occupying the lowest energy (band) state, the d's could form a Bose Einstein Condensate (BEC). At the time this suggestion was made, confusion about its relevance resulted [14] because it was widely believed that BEC's could form only at very low temperatures, as opposed to a situation in which they are induced (as in the case of laser-cooling of alkali vapors) dynamically through the presence of externally applied forces. In addition, the suggestion that IBS's could be involved in cold fusion was not widely publicized for two reasons: 1) The experiments were not widely believed to be valid; and 2) Perceptions about the limitations of conventional energy band theory.

Over the years, the associated IBST has evolved considerably. It has, in fact, been used to provide a number of predictions about excess heat in cold fusion that were subsequently observed. In responding to the critics of the theory, the author has shown that the basis of the criticism, associated with limitations of energy band theory, reflect biases that are the result of the approximate justification for the theory and the way this justification is usually presented. In addressing this problem, the author has developed a generalization of the conventional theory, based on a procedure (referred to as Generalized Multiple Scattering Theory), that provides a framework for both generalizing conventional energy band theory and

for understanding how, in the context of conventional physics, excess heat in cold fusion, through coherent forms of nuclear fusion, in which the wave-like features of "particles" associated with conventional energy band theory can be formally re-expressed in a manner that quantifies how the associated effects can occur without high energy particle emission.

The paper is organized in the following way. In the next section, an overview of IBST is presented that provides important background information about the new physics that is assumed in the associated description, as well as effects that the theory has predicted. In the following section, the key features of Generalized Multiple Scattering Theory are reviewed. In the final section, an explanation is provided of how nuclear reactions in PdD can take place, again, based on the conventional laws of physics.

2. Overview Of The Ion Band State (IBST)

Through the associated ion band state theory (IBST) [6, 7, 8, 9], a number of effects were predicted that were subsequently observed experimentally, including the following:

1. That ^{4}He is created when excess heat is produced at appropriate levels that account for the heat through a nuclear reaction [15, 16, 17, 18];
2. That the ^{4}He is found in an unanticipated location, outside heat-producing electrodes [15, 16, 17, 18];
3. That there is an apparent requirement that for the effect to occur, "high-loading" (defined by the limit $x \rightarrow 1$ in PdD_x) is necessary [5]; and
4. That the effect occurs without the emission of any high energy particles or radiation [4, 15, 16, 17, 18].

The "high-loading" limit, which is emphasized in this paper, applies to electrolysis experiments. In gas-loading experiments [6] involving nm powders of Pd, "high-loading" might not be required as a result of interfacial chemistry effects.

In responding to the critics of the IBST, the author identified important effects, involving particle indistinguishability, degeneracy, and band theory that can be applied not only to the PdD fusion problem but in more general terms. In particular, although energy band theory is usually formulated in terms of the semi-classical limit of a single-particle, eigenvalue problem, as it applies to infinitely-repeating periodic systems; it was actually derived by Bloch through a formalism (multiple scattering theory) that has more general applicability.

In fact, although conventional multiple scattering theory is defined in terms of the scattering properties of single particles with an array of scattering centers, it can be generalized [19]," to situations involving arbitrary collisions between arbitrary numbers of particles in many-body systems. Although the resulting equations are usually so general that they are intractable, in a limited set of circumstances, involving finite, periodic lattices, they can be used to establish a hierarchy of processes, involving different rates of reaction, as a result of approximate translational invariance. Within this context, conventional energy band theory can be derived as a limiting situation associated with the lowest energy excitations of these kinds of lattices.

These occur through perfectly resonant forms of interaction, involving rigid translations of the lattice in situations in which fluxes of particles into and away from the region of space occupied by the lattice vanish. Implicit in this limit is the importance of approximate translation symmetry. In fact, because it is never possible to determine the precise location of the boundaries of a lattice, it is never possible to tell precisely where it begins and ends and whether or not its center-of-mass (CM) is in motion or at rest. Implicitly, this result is associated with a form of Galilean relativity: it is never possible to tell if an outside observer is in motion or at rest, relative to a periodic (or approximately periodic), finite array of atomic centers and electrons. As a result of this symmetry, a huge degeneracy exists, associated with rigid translations, in which the separations between all of the particles remain fixed.

In fact, this symmetry, which also is a (somewhat trivial) form of gauge symmetry, provides a mechanism for the relative momentum between one particle and a second particle to change arbitrarily (as a result of generalized forms of Umklapp processes, which can also be viewed as forms of broken gauge symmetry) at a point through implicit forms of coupling involving the electromagnetic field during

collision processes. (This is the basis of the Mossbauer effect.) In more general terms, the associated many-body configurations, associated with finite, ordered lattices provide a environment for particle-particle collisions that are dominated by the effects of particle indistinguishability and degeneracy.

This fact provides justification for a number of important, new results, associated with collisions in solids that have not been widely appreciated. In particular, at an early stage, our suggesting that if d's occupy IBS's (and form what we referred to as Bose Bloch Condensate) it might be possible for new forms of fusion to take place was widely criticized [14], based on the observation that conventional band theory only applies in situations in which details about particle-particle interactions can be ignored. In fact, although in conventional band theory, this appears to be the case, implicitly, an important reason for this is that a semi-classical limit of the associated physics has been widely used, and details about the underlying many-body physics have been ignored. In this context, degeneracy (or near-degeneracy), resulting from particle indistinguishability and periodic order has important implications. In particular, as in the Mossbauer effect, through a real effect, implicit in the symmetry associated with rigid lattice translations that preserve periodic order, it is possible for a lattice to "recoil" elastically, as a whole, in response to a collision at a point. In the generalization of band theory [19] to many-body, finite systems, the same symmetry is invoked and leads to a huge degeneracy. Because indistinguishable particles are involved in these systems, implicitly, additional degeneracies are also present.

The combined effects provide a means for particles to have appreciable overlap at many, periodically displaced "points" (as discussed below), simultaneously, for finite periods of time, in a manner that can result in new forms of collisions in which momentum is transferred from the locations where overlap can occur, rigidly to the lattice as a whole. When these idealized forms of motion are initiated by collisions resulting from the overlap between d's in IBS's, they can result in forms of coupling that can cause nuclear fusion to take place in which small amounts of momentum and energy from many different locations are transferred coherently to the solid as a whole and subsequently transferred to many different particles in a cooperative fashion. As a consequence, in agreement with experiment, the associated nuclear energy is predicted to be released without high-energy particles.

Because the theory assumes the underlying physical situation involves collisions that can arise from very similar configurations that are degenerate or nearly degenerate, the resulting process, if it occurs, is very different from processes that involve collisions in free space. Furthermore, as opposed to the situation in free space, where, in order for fusion to occur, d's are "forced" to occupy a common volume (by over-coming a Coulomb Barrier), in the situation in the solid, effectively, a form of decay can occur, in which d's not only are allowed to have appreciable overlap (in order to minimize energy) by occupying IBS's, but ^{4}He can be created (also in an IBS form). Thus, as opposed to being forced to occupy a common volume externally (as in free space) by requiring the d's to have high velocity, through quantum mechanical effects the solid can cause the d's to do this, without requiring that any of them have appreciable velocity.

An important point is that the Bose exchange symmetry of d's, as well as the possible processes associated with the underlying periodic order (and the potential, coherent forms of interaction that can occur when *d's* occupy IBS's) are associated with a very particular limit, involving low energy (ion band state-like) fluctuations in charge, in which only a very small concentration of *d's* ($\sim 10^{-4}$ per unit cell) is involved. It is also important that this limit, which is consistent with the electronic structure of the relevant structure [5, 20], which involves highly loaded PdD (defined by PdD_x, $x \rightarrow 1$), is predicted to involve a dynamical process that actually minimizes the underlying Coulombic repulsion associated with *d-d* fusion [8].

In the lowest energy configurations, the associated collisions release momentum and energy at the boundaries of the lattice. An important point is that the associated degeneracy (and near degeneracy) and resulting overlap and interaction are coupled to each other through interaction with the lattice (and, implicitly, its electronic structure). In this context, as opposed to over-coming the conventional "Coulomb Barrier" through processes that are initiated when localized particles possessing a well-defined

(nearly constant) relative momentum at high velocity collide at a point, a more sophisticated (implicitly time-dependent) "Barrier" is involved.

Because the underlying dynamics is associated with rigid lattice recoil, the associated problem of overcoming the "Barrier" (as outlined below) is related to crystal size and a number of additional environmental factors. In the case of PdD, a key result (that is also observed [5, 20]) involves the prediction that a near full-loading ($PdD_{1\pm\delta}$, $\delta \to 0$) condition is required for excess heat to be created. (A new result is the prediction that this near full-loading condition is required because approximate periodic order is necessary for the d's to occupy band states and, because of the anti-bonding characteristics of the electronic structure in PdD, which is responsible for the d's behaving as ions.)

Because the reaction is initiated from a state in which interacting *d's* possess Bose exchange symmetry, details about the electromagnetic interaction are important far from the location of the reaction, and (as opposed to the situation in the more common ($d + d \to {}^3H + p$ and $d+d \to {}^3He+n$) fusion reactions, the electromagnetic and nuclear interactions are not separable. (In the case of the "rarely-occurring," $d+d \to {}^4He+\gamma$, reaction a similar lack of separability between electromagnetic and nuclear interactions also takes place.) Because of this fact and because of the large degeneracy and overlap with many-body configurations in which the final state product possesses ^{4}He, through the IBST, it was predicted [7, 8, 9, 21] (prior to observation) that (in order to minimize energy), the fusion process that creates this product in a solid (as opposed to ^3H and protons or ^3He and neutrons) would be dominant in the heat-producing reactions. Because of the requirement that periodic order be present, through the theory, it was suggested that this product would be initiated through the occupation of transient ^4He in IBS's that would be neutralized at the boundaries of the solid, where it would be released in atomic form (again prior to and in agreement with experiment [15, 16, 17, 18]).

In the next two sections, it is demonstrated that appreciable reaction rates for fusion of the form, $d+d \to {}^4He + 23.8\ MeV$ (in which the *23.8 MeV* is dispersed throughout the solid), can occur, near full-loading in PdD. Because the associated rates result from the lowest energy excitations of the lattice, they can be estimated using the generalization of multiple scattering theory [19, 22]. In the resulting limit, overlap between *d's* in IBS's is allowed to take place inside the lattice near nuclear dimension (defined when the separations between the CM's of *d's* become vanishing-ly small on the length scales associated with electromagnetic interaction in the lattice) as a result of discontinuous changes in momentum (wave function cusps) at the locations where this takes place. (These kinds of abrupt changes in momentum are allowed to take place, as a consequence of broken gauge symmetry, in which the gauge associated with the vector potential is allowed to shift by a constant amount in one region—the nuclear region, where nuclear overlap is allowed to take place—relative to the rest of the solid) through rigid translations of the lattice. Nuclear reaction (which, technically occurs outside the lattice) involves a transition at these locations through processes associated with *d+d* fusion that can be modeled (in a manner that is consistent with multiple scattering theory and the constraints associated with a lower bound on reaction rate) through a shift in the zero of energy of the lattice and the coherent transfer of momentum from the reaction to the solid as a whole.

3. Generalized Multiple Scattering Theory And Its Relationship To Band Theory

The wave-like behavior of quasi-particles that occurs in the conventional energy band theory formalism can be rigorously understood from wave-particle duality effects that result from a form of Galilean Relativity. In particular, for a solid possessing total mass M_T, each possible velocity ($\vec{V}_j$) associated with the relative motion of an observer and a solid that is stationary involves a different center-of-mass momentum $\vec{P}_{cm,i} = M_T \vec{V}_j$, which in turn can be used to define a particular wave-vector,

$$\vec{k}_i = m\frac{\vec{P}_{cm,i}}{M_T\hbar}, \tag{1}$$

for each particle possessing mass *m*. Perfect resonance [23] occurs when the possible values of the wave-vector $\left(\vec{k}_i\right)$ are used to define the energies $\varepsilon_i = \varepsilon\left(\vec{k}_i\right)$ of possible excitations of the system, and through two requirements [19]: 1) That the set of allowable wave-vectors be restricted to the first Brillouin zone; and 2) That each value of $\varepsilon\left(\vec{k}_i\right)$ possess a discrete (invertible) Fourier transform, associated with the (finite) set of Bravais vectors $\left(\vec{R}_n\right)$ that is used to define the lattice:

$$\varepsilon\left(\vec{k}_i\right) = \sum_n \varepsilon_n e^{i\vec{k}_i\cdot\vec{R}_n}, \tag{2}$$

$$\varepsilon_n = \frac{1}{N_{cell}}\sum_i \varepsilon\left(\vec{k}_i\right)e^{-i\vec{k}_i\cdot\vec{R}_n}, \tag{3}$$

where N_{cell} is the number of unit cells in the lattice.

The many-body wave function of each excitation can be expressed through a generalized form of Bloch's theorem [19, 22], associated with the band energies and wave-vectors used in equations (2) and (3). As a consequence of these equations and the relationship between the wave-vectors and the large number of possible Galilean transformations, associated with rigid translations, it follows that an implicit degeneracy is present in which each value of $\varepsilon\left(\vec{k}_i\right)$ satisfies

$$\varepsilon\left(\vec{k}_i\right) = \varepsilon\left(\vec{k}_i + \vec{G}_n\right) \tag{4}$$

and is associated with a situation in which the lattice as a whole is allowed to move rigidly with a CM momentum $\vec{P}_{cm,n} = \hbar\vec{G}_n$, defined by one of the reciprocal lattice vectors $\vec{G}_n$.

Although equation (4) holds only in the absence of perturbations in the interior of the solid and at its boundaries, in fact, on some time scale, it actually applies for all of the particles and low-lying excitations (which may involve quasi-particles, including phonons) in the system. As a result, a huge degeneracy exists. In practice, perturbations, which break this symmetry, always exist, and for this reason, usually, the only ones that have an impact on the dynamics appear to be the ones that involve electrons that occupy energy band states or phonons. An important point is that implicitly the degeneracy associated with equation (4) potentially can result in a situation in which the energy of a perturbation results in a coupling between many different particles and/or states, each involving a different CM momentum, that preserves periodic order in the interior of the solid.

In situations in which d's occupy IBS's, provided the crystal lattice is sufficiently large, values of $\vec{P}_{cm,n} = \hbar\vec{G}_n$ can be significantly larger than the momentum that is required to initiate a nuclear reaction. For this reason, provided overlap between d's can take place over length scales associated with nuclear reaction (and we shall see that this can occur when the relative momentum between interacting d's changes sufficiently rapidly over short distances), fusion can occur.

When d's interact and undergo fusion by occupying IBS's, the degeneracy associated with equation (4), which is the basis of Bloch's theorem, leads to forms of overlap and interaction which have no counterpart in conventional fusion in free space, where a semi-classical picture applies in which momentum is transferred only between two particles and is constrained to change slowly. Because in the situation involving energy band states, the associated change in momentum involves a form of rigid lattice recoil, it can provide a mechanism for transferring energy and momentum, non-locally, in an

elastic fashion that implicitly leads to a coupling between many particles. For this reason, potential fusion reactions that can be initiated from this kind of process need not involve particles that have high energy and momentum.

A lower bound for potential nuclear reactions that can result from the associated IBS picture can be estimated using the logic that was used, involving generalized multiple scattering [19, 22], to extend conventional energy band theory to situations involving finite lattices. The associated argument involves an analysis of the time evolution of the overlap between the ground state (GS) many-body wave function $\Psi_{GS}(r_1,.....,r_n,t)$ with the comparable wave functions of the lowest lying excitations. The first step in the analysis is the observation that as a function of time t, because $\Psi_{GS}(r_1,.....,r_n,t)$ describes the GS, it is required to have minimal coupling with outside processes, and its overlap with any other many-body state $\Psi'(r_1,.....,r_n,t)$ must be minimized and remain constant; while, for a sufficiently large solid, the GS and the lowest lying excitations of the solid, are required to possess the symmetry associated with rigid lattice translations, defined by equation (1). A requirement for this to occur is:

$$\frac{\partial <\Psi'/\Psi_{Gs}>}{\partial t} = \iiint d^3r_1...d^3r_n \frac{\partial(\Psi'^{*}\Psi_{GS})}{\partial t}$$
$$= -\int d^3r \nabla \bullet <\Psi'/v(r)/\Psi_{GS}> + <\Psi'/\frac{V-V'}{i\hbar}/\Psi_{GS}> = 0, \quad (5)$$

where terms in the second equality are defined by the many-body Schroedinger equations of Ψ' and Ψ_{GS}.

In general, the associated integrations are unrestricted. To extend energy band theory to finite lattices, it is appropriate to consider situations in which minimal overlap in "bulk regions" (associated with equations (1)-(4), takes place. In this situation, the unrestricted integrations over all of the coordinates in the multi-dimensional integral, term by term, can be restricted to regions in the bulk, based on the criteria that to find a possible GS, the associated overlap between this state and other states in the bulk region is required to be minimized. In this limited context, by restricting states to have minimal overlap with Ψ_{GS}, additional restrictions are imposed on Ψ_{GS} (subject to the implicit assumption that, in general, at the boundaries of the bulk region, possible discontinuities in the gradient and vector potential, are allowed to take place). Then, the analysis associated with extending band theory to finite lattices proceeds by restricting the multi-dimensional integrations in equation (5), exclusively to the bulk region. In the more general situation, considered here, rate expressions can be derived for different regions (bulk and non-bulk), associated with the requirements that charge be conserved (in bulk regions) or not conserved (in non-bulk regions), subject to the constraint that in bulk regions states are required to have minimal overlap with Ψ_{GS}. Also, in equation (5), $\langle\Psi'|v(r)|\Psi_{GS}\rangle$ is the matrix element associated with the (off-diagonal) contribution to the (many-body) particle velocity operator *v*, defined by its overlap with the states Ψ' and Ψ_{GS}:

$$<\Psi'/v(r)/\Psi_{GS}> = \sum_j \iiint d^3r_1..d^3r_n \delta^3(r-r_j)\frac{1}{m_j}\frac{\hbar}{2i}\left(\left[\Psi'^{*}\nabla_{r_j}\Psi_{GS} - \nabla_{r_j}\Psi'^{*}\Psi_{GS}\right] - \frac{e_j}{c}\Psi'^{*}A_{eff}(r_j)\psi_{GS}\right), \quad (6)$$

where $A_{efi}(r)=(A(r)+A'(r))/2$ is the arithmetic mean between the vector potential A'(r) associated with the state Ψ' and the comparable vector potential A(r), associated with the state Ψ_{GS}, and the final term in equation (5) is defined by the difference between the many-body potential energies associated with states Ψ' and Ψ_{GS}. . In particular, this last term, is given by

$$< \Psi' / \frac{V - V'}{i\hbar} / \Psi_{GS} > = < \Psi' / \frac{V_{em} - V'_{em}}{i\hbar} / \Psi_{GS} > + < \Psi' / \frac{V_s - V'_s}{i\hbar} / \Psi_{GS} >, \quad (7)$$

where $< \Psi' / V_{em} - V'_{em} / \Psi_{GS} >$ is the difference in electromagnetic potentials associated with coupling between the vector potentials A'(r) and A(r),

$$< \Psi' / V_{em} - V'_{em} / \Psi_{GS} > = \int d^3 r \frac{\left(A(r) - A'(r)\right)}{c} \cdot J(r), \quad (8)$$

defined by the associated current J(r),

$$< \Psi' / J(r) / \Psi_{GS} > = \sum_j \iiint d^3 r_1 .. d^3 r_n \delta^3 (r - r_j) \frac{e_j}{m_j} \frac{\hbar}{2i} \left(\left[\Psi'^* \nabla_{r_j} \Psi_{GS} - \nabla_{r_j} \Psi'^* \Psi_{GS} \right] - \frac{e_j}{c} \Psi'^* A_{eff}(r_j) \psi_{GS} \right),$$

and [in equation (7)], the remaining contribution to the difference in potential energy is defined by any change in electrostatic and other (for example, nuclear) contributions to the energy, associated with the transition from Ψ' (where the non-electro-dynamic portion of the potential energy is V_s') to Ψ_{GS} (which has a corresponding non-electro-dynamic potential energy V_s).

When Ψ_{GS} has minimal coupling to the bulk, equation (5) holds identically, outside the bulk, provided the total internal flux of all particles into and away from the bulk region also vanishes. Thus, if the flux of particles, across all boundaries in the bulk vanishes, and the energies of the different states are the same within the bulk region, it follows from equation (2) that,

$$\int d^3 r \nabla \bullet < \Psi' | v(r) | \Psi_{GS} > = \int_{\partial V} dS \, \hat{n} \bullet < \Psi' | v(r) | \Psi_{GS} > = (i\hbar)^{-1} \iiint_V d^3 r_1 .... d^3 r_n \Psi'^* (V - V') \Psi_{GS} \quad (9)$$

where the integration in the final term can either extend only over the bulk region or regions outside the bulk, and the surface integral (associated with v(r)) extends over the boundary of the region where the contribution to the matrix element involving *V-V'* is evaluated. When the integration only includes the bulk region, and its boundary, when particle flux vanishes, $\int_{\partial V} dS \, \hat{n} \cdot < \Psi' / v(r) / \Psi_{GS} > = 0$, and the bulk contribution to the matrix element involving *V-V'* vanishes. This fact is used to establish the extension of band theory to finite lattices [19, 22]. In general, this surface integral may include separate contributions from regions where *v* may become discontinuous (which are allowed to occur whenever *V-V'* becomes singular). (As discussed below, an idealized limiting case, associated with locations where nuclear reaction can occur in the fusion problem, involves allowing for such discontinuous behavior—through wave function cusps.) equation (5) vanishes identically whenever the energies associated with Ψ_{GS} and Ψ' are the same. This means equation (9) can also be used to evaluate the rate R for any reaction that is initiated from an initial state possessing a particular E. In particular, from the Lippman-Schwinger equation, it follows [19] that each term in the expression for R conserves energy and involves the square of a matrix element involving *V-V'* that (as a result of equation (7) and Gauss' law) can be represented in terms of a surface integral

$$\int_{S_\alpha} d^2 r_\alpha < \Psi_o / v(r_\alpha) / \Psi_{exact}(C_F) >$$

involving a different (exact) representation of a possible final state $\Psi_{exact}(C_F)$, the initial state Ψ_o, and the velocity operator $v(r_\alpha)$:

$$R \equiv \frac{1}{\tau} = 2\pi\hbar \sum_F \delta\left(E - E_{exact}\left(C_F\right)\right) / \sum_\alpha \int_{S_\alpha} d^2 r_\alpha < \Psi_o / v\left(r_\alpha\right) / \Psi_{exact}\left(C_F\right) >|^2 , \tag{10}$$

where τ is the lifetime of the state.

4. Nuclear Reactions in PDD

As noted in the last section, in the situation associated with fusion, we are suggesting that the reaction occurs when a small concentration (<~10^{-4}) of d's become wave-like by occupying IBS's, and ^{4}He is created (in bulk regions) in wave-like IBS form [8, 9, 19, 24]. When this occurs, a small fraction of a potential reaction occurs in each unit cell. The associated picture can be justified rigorously by noting that as a consequence of the generalization of energy band theory to situations involving finite lattices [19, 22], the generalized form of Bloch's theorem applies in which Φ_{GS} and Φ' possess Bloch symmetry with respect to Bravais lattice vector translations involving the CM coordinates of the d's and the separation coordinate $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$ associated with the distance between two potentially interacting d's (located at $\vec{r}_1$ and $\vec{r}_2$). As a consequence, nuclear overlap is allowed to take place at the N_{cell} locations (associated with different Bravais lattice vectors $\vec{R}_N$) where $\left|\vec{r}_{12} - \vec{R}_N\right| = 0$, which means that $\Delta E_{zero} = \Delta mc^2 / N_{cell}$, where Δmc^2 =23.8 MeV is the energy that is released from the change in mass in the $d + d \rightarrow {}^4He$ reaction.

The situation that is of interest in the fusion problem occurs when the zero of momentum is allowed to change at these locations. (Technically, since the bulk region is required to be neutral (Chubb, 2005A), the nuclear region is located outside this region since a net accumulation of charge occurs at the locations where nuclear reactions are allowed to occur.) In particular, the zero of momentum of the bulk is allowed to change when it is assumed that a rigid translation of the nuclear region, relative to the bulk, is allowed to take place. This occurs when the gauge (defined as the gradient $\nabla\Phi$ of the gauge function Φ) associated with A_{eff} shifts by the same constant amount at each location of the boundary between the bulk and nuclear regions. (As noted above, nuclear fusion reactions, resulting from such a change, occur through a broken gauge symmetry.)

In fact, to establish a finite, lower bound for nuclear reaction rate, it follows that interactions in the bulk should be minimized (and the right and left sides of equation (9) vanish identically when they are restricted to the bulk). For this reason, in this limit, these forms of rigid lattice recoil are required. Furthermore, it also follows as a result of energy conservation and the fact that the surface integral (involving the flux) can be related to the change in kinetic energy that the lowest energy finite reaction rate associated with nuclear reactions occurs when the only non-vanishing contributions to the total flux occur at the boundary of the nuclear region and result from the change in the zero of energy ΔE_{zero} associated with the change in mass that results when two d's form ^{4}He and the d's have overlap in the nuclear regions:

$$\int d^3 r \nabla \bullet < \Psi' / v\left(r\right) / \Psi_{GS} > = \int_{\substack{nuclear \\ boundary}} dS\, \hat{n} \bullet < \Psi' / v\left(r\right) / \Psi_{GS} > = \iiint_{\substack{nuclear \\ region}} d^3 r_1 .... d^3 r_n \Psi'^* \left(V - V'\right) \Psi_{GS}$$
$$= \frac{i}{\hbar} \Delta E_{zero} \iiint_{\substack{nuclear \\ region}} d^3 r_1 .... d^3 r_n \Psi'^* \Psi_{GS} = \frac{i}{\hbar} \frac{\Delta mc^2}{N_{cell}} O_{nuc} \tag{11}$$

Here, the right-side of the first equality involves a surface integral that includes possible (constant) changes in the effective vector potential A_{eff} that result from elastic, recoil processes (which can be

viewed as changes in the gauge of A_{eff} that occur at the boundaries of the bulk) in which the lattice moves rigidly through a constant shift of the zero of momentum of the bulk, relative to the nuclear region and regions outside the solid. This expression as well as the expression on the right-side of the second equality involve contributions only from the nuclear region (although, in principle, they could involve contributions from other regions, that are external to the solid) because the associated analysis applies for situations involving a lower limit for reaction rate. In the final equality, O_{nuc} denotes the overlap between Ψ' and Ψ_{GS} in the nuclear region.

Equations (9) and (10) can be used to establish a bound, based on the assumption that nuclear overlap can take place. It follows that when Ψ' and Ψ_{GS} involve IBS's, this can occur provided the bulk region remains near its GS when energy (and system perturbations) are minimized in situations involving near full-loading. In this limiting situation (defined by PdD_x , $x = 1 \pm \delta$), small variations $\delta\left(<\sim 10^{-4}\right)$ in loading are expected to induce fluctuations in the charge [22] in each unit cell involving a highly polarized, anti-bonding change in electronic structure [23] in which the electron associated with each entering D-atom effectively dissociates from the corresponding (*d*) nucleus. Because near the GS, *V-V'* in the bulk region vanishes, asymptotically, Ψ' and Ψ_{GS} can be treated as if they are in perfect resonance with the solid. Then, the generalized band theory, associated with equations (1)-(4), which includes the generalized form of Bloch's theorem [19, 22], applies and can be used to model the behavior of the d's associated with the fluctuation (through the occupation of IBS's).

In addition, in this, near-GS limit, when δ is sufficiently small, Coulombic repulsion, in the bulk, between the d's associated with the fluctuations in loading asymptotically vanishes, and since no change in the potential takes place in this region, the associated many-body wave functions (Ψ' and Ψ_{GS}) can be treated as products of single-particle (IBS) wave functions. This fact can be used to construct (Bose symmetric) many-body wave functions that can be used in equation (10) to estimate a bound for R [24] (as discussed below). Implicitly, because the associated rate involves rigid forms of lattice recoil that occur when pairs of d's have overlap, d-d interactions, in which momentum is allowed to change discontinuously, are allowed to occur.

The associated interaction (which involves a many-body effect) asymptotically occurs at locations where the separation between the CM of one d and the CM of a second d vanishes. This can be modeled by allowing for singular behavior (on the length scales associated with electrostatic interaction) in the d-d Coulomb potential in bulk regions that asymptotically approach the locations where nuclear overlap takes place. In order to include these interactions, in the bulk region, two-particle wave functions can be used that possess Bloch symmetry, with respect to variations in the CM of each d that is injected during the fluctuations in loading.

Here (as a consequence of the generalized form of Bloch symmetry), the CM dependence of the 2-deuteron wave function for each pair of d's can be treated using a single-particle IBS, possessing Bloch symmetry; while in order to minimize the Coulombic repulsion between a pair of d's, the dependence on the separation $\vec{r}_{12}$ between the CM's of different d's is treated using a second, single-particle wave function that is also an IBS (and possesses Bloch symmetry) [23]. As a consequence, singular behavior and nuclear reaction are allowed to take place at each periodically equivalent location $\left|\vec{r}_{12} - R_n\right| = 0$, associated with a different Bravais lattice vector R_n.

In principle, because perfect resonance occurs in the bulk, the two particle wave function $\Psi\left(\vec{r},\vec{r}_{12}\right) = \Phi_{cm}\left(\vec{r}\right)\Phi_s\left(\vec{r}_{12}\right)\left(\vec{r} = \frac{1}{2}\left(\vec{r}_1 + \vec{r}_2\right)\right)$, associated with the CM and separation single particle wave functions ($\Phi_{cm}\left(\vec{r}\right)$ and $\Phi_s\left(\vec{r}_{12}\right)$, respectively), in bulk regions, can be determined from an effective, two particle Hamiltonian *H* of the form,

$$H \equiv \{-\frac{\hbar^2}{4m_D}\nabla_r{}^2 + U_{lattice}(r)\} + \{-\frac{\hbar^2}{m_D}\nabla_{r_{12}}{}^2 + \sum_j \frac{e^2}{N_{cell}\,|\vec{r}_{12} - R_j|}\}, \tag{12}$$

subject to the implicit requirements that since H is bounded and periodic with respect to Bravais lattice vector translations, the functions $\Phi_{cm}(\vec{r})$ and $\Phi_s(\vec{r}_{12})$ are both required to possess Bloch symmetry ($\Phi_{cm}(\vec{r}+R_n) = e^{ik\bullet R_n}\Phi_{cm}(\vec{r})$, and $\Phi_s(\vec{r}_{12}+R_n) = e^{ik\bullet R_n}\Phi_s(\vec{r}_{12})$). Here, in equation (12), $U_{lattice}(r)$ is an effective single particle (periodic) potential associated with the interaction of the charges in the lattice with an effective quasi-particle (a "di-deuteron") involving two d's that occupy an IBS, at the location of their CM, and the final term in the second line is the two particle potential that results (through self-interaction) from d-d Coulombic repulsion between two d's that also both occupy IBS's. Here, the separation variable wave function $\Phi_s(\vec{r}_{12})$ is normalized so that its integral over the entire crystal is unity. As a consequence, the associated "quasi-particle" has an effective charge of e/N_{cell} (which is the reason the factor of N_{cell} appears in the denominator of the expression associated with the d-d Coulombic repulsion).

The requirement that H be bounded is satisfied when $\nabla^2\Phi_s(\vec{r}_{12})$ becomes appropriately singular (through discontinuities in the local momentum $(\hbar/i)\nabla\Phi_s(\vec{r}_{12})$) at the locations where the Coulomb repulsion term in equation (12) becomes singular in such a way that the two singularities cancel each other. This condition is satisfied when $\Phi_s(\vec{r}_{12})$ is allowed to have a suitable cusp (a discontinuity in its gradient) whenever $/\vec{r}_{12} - R_j/ = 0$. Because no perturbation occurs in the bulk region (and $\int_{Bulk} d^3r\nabla\bullet < \Psi'/v(r)/\Psi_{GS} > = 0$), effectively, H can be modeled as a self-adjoint, two-particle Hamiltonian.

Because a bound for R is sought, $\Psi(\vec{r},\vec{r}_{12})$ can be assumed to minimize H. This can be accomplished by extending the variational procedure that Hylleraas [25] used to find the two-electron wave functions in the helium atom, to a situation involving IBS's. Then, it is possible to find an approximate form for $\Psi(\vec{r},\vec{r}_{12})$. In particular, a particular functional form for $\Phi_s(\vec{r}_{12})$ is used, involving particular variational parameters, which are approximately determined by minimizing the energy, and, in analogy with the procedure that Hylleraas used, the cusp in this functional form is introduced by requiring that it depend on $/\vec{r}_{12}/$ [23]. A key feature of this calculation is that $\Phi_s(\vec{r}_{12})$ is assumed to be a periodic function with respect to Bravais lattice translations. For each value of $\vec{R}_n$, the assumed functional form for $\Phi_s(\vec{r}_{12})$ is

$$\Phi_s(\vec{r}_{12} - R_n) = \frac{A\left[1 + b\,sin\left(\pi/\vec{r}_{12} - R_n/(4r_{sc})\right)\right]}{1+b} \qquad /\vec{r}_{12} - \vec{R}_n/ < 2r_{sc}\,. \tag{13}$$
$$= A \qquad\qquad /\vec{r}_{12} - \vec{R}_n/ \geq 2r_{sc}$$

Here, it is also assumed that a suitable screening length r_{sc} = *0.156 Å = 0.1* Wigner Seitz radius (R_{WS}) applies (that is required to be significantly smaller than R_{WS}), A is a normalization constant, and b is a variational parameter.

In Chubb and Chubb [26]), a relationship between N_{cell}, r_{sc}, and b was inferred, based on an approximate energy minimization calculation and the assumption that b<1. A more precise relationship involves the "cusp condition." When this condition and energy minimization are both used (as shown below), b can be explicitly evaluated, and it is found that this last assumption (that b<1) is not valid. This

last calculation also establishes a relationship between N_{cell} and r_{sc}. Here, the "cusp condition" refers to a cancellation between the singular term

$$-\frac{\hbar^2}{M}\nabla_x{}^2\Phi_s(\vec{x}) \to -\frac{Ab}{1+b}\frac{\hbar^2}{M}\frac{\pi}{4r_{sc}}\times\frac{1}{/\vec{x}/};$$

associated with the discontinuity in

$$\nabla\Phi_s(\vec{x}) = -\lambda\hat{x}\frac{Ab\cos(\lambda|\vec{x}|)}{1+b},\ \lambda=\frac{\pi}{4r_{sc}}$$

from the kinetic energy contribution [in equation (12)] involving the separation variable with the comparable singularity $\left(e^2/N_{cell}\right)\left(\Phi_s(\vec{x})/|\vec{x}|\right)$ in the Coulombic repulsion contribution that results each time $/\vec{r}_{12}-\vec{R}_n/=/\vec{x}/\to 0$. This form of cancellation has been employed routinely, in bound state systems, to provide realistic wave functions, for example, in atomic and molecular physics [27] and in quantum Monte Carlo calculations by Reynolds *et al.* [28] and Umrigar *et al.* [29]. The "cusp condition" leads to a relationship between b, r_{sc}, and N_{cell}:

$$N_{cell} = \frac{M_D}{M_e}\frac{r_{sc}}{a_e}\frac{4}{\pi}\frac{1}{b} = \frac{8439\ r_{sc}}{b} = \frac{1319}{b}, \tag{14}$$

where $a_e = \hbar^2/m_e e^2$ is the Bohr radius of an electron, and m_e is the mass of an electron.

As mentioned above, by imposing the "cusp condition" [equation (13)] and by minimizing H (with respect to b) it is possible to evaluate b. This is accomplished by minimizing the energy functional

$$\frac{\int\Phi_s{}^*H_{12}\Phi_s d^3r_{12}}{\int\Phi_s{}^*\Phi_s d^3r_{12}},$$

where

$$H_{12} = -\frac{\hbar^2}{m_D}\nabla_{r_{12}}{}^2 + \sum_j\frac{e^2}{N_{cell}{}^2/\vec{r}_{12}-R_j/}.$$

This procedure leads to a second relationship between N_{cell}, b, and r_{sc}:

$$\begin{aligned} N_{cell} &= \left(\frac{M_D}{M_e}\right)\left(\frac{r_{sc}}{a_e}\right)\frac{\left[-16\pi+\frac{128}{\pi}+\left(8\pi-\frac{96}{\pi}\right)b\right]}{\left(16-8\pi+\left(8\pi-16-\frac{2\pi}{3}\right)b\right)}. \\ &= \left(\frac{M_D}{M_e}\right)\left(\frac{r_{sc}}{a_e}\right)\frac{[-9.522-5.425\,b]}{(-9.133-11.538\,b)} \end{aligned} \tag{15}$$

When equation (13) is substituted into equation (15), the resulting expression leads to a quadratic equation that can be used to determine b

$$\begin{aligned} 0 &= (2\pi^2-24)b^2+(48-8\pi-4\pi^2)b+8\pi-16 \\ &\cong -4.261b^2+4.060\mathrm{b}+9.133 \end{aligned}. \tag{16}$$

Equation (16) has two roots. One of these has a positive value; while the other one is negative. Because N_{cell} is positive, as a result of the cusp condition [equation (13)], only the positive root applies

$$b = 2.016\,. \tag{17}$$

By substituting equation (17) into equation (13), it is possible to find a value for

$$N_{cell} = 6504.000 \times r_{sc} = 654\,. \tag{18}$$

This last calculation provides an approximate bound for N_{cell}. A different estimate, based on the requirement that momentum from a potential nuclear reaction is coherently transferred through a rigid translation in a particular direction, leads to a comparable, but larger, bound [22], $N_{cell} \geq 3 \times 10^3$.

Both of these estimates provide potential bounds for N_{cell} that are required for fusion to occur when they are initiated through IBS occupation. However, neither estimate includes specific information about the time-scale associated with the reaction. In Chubb [19, 30], a model (based on a potential triggering mechanism) is presented that suggests the necessary time that is required (in optimal situations) for this bound to apply is ~7 ms. (Note the following correction: $i_1\Delta t_1 = i_2\Delta t_2 = 4\pi N_{vert} / a \,|\, eE \,| = t_{trig} = 3.03\ \mu s$, on the final page of both references, should be replaced with the expression, $i_1\Delta t_1 = i_2\Delta t_2 = 4\pi N_{vert}{}^3\ \hbar / a \,|\, eE \,| = t_{trig} = 0.68\ ms$). This may induce changes in the lattice structure that could invalidate the assumption that the bulk remains in its GS. In Chubb [30, 31], a more refined estimate (involving a triggering time of ~7 s) is given, $N_{cell} \geq 3 \times 10^6$, that ensures that the bulk solid remains in its GS.

When a still higher bound for N_{cell} ($\geq 3 \times 10^9$) is assumed, the resulting value of E_{zero} (≈ 0.008 eV) associated with equation (10) is sufficiently small that the contribution in each unit cell to the energy of the associated perturbation

$$\iiint\limits_{\substack{nuclear \\ region}} d^3r_1 \ldots d^3r_n \Psi'^{*}(V - V')\Psi_{GS}$$

is less than the energy that is necessary to excite the lowest energy (0.02 eV) optical phonons in PdD. When this last bound applies, equation (10) reduces to a Fermi Golden Rule estimate of R, which was used previously [24]. This estimate is based on the assumption that an implicit selection rule applies (in which initial and final states involve bosons, constructed from proton-neutron pairs), and, as a consequence, the nuclear portion of the reaction can be modeled, using the algebraic properties and combinatorics of many-body wave functions that are appropriate for indistinguishable bosons. These many-body wave functions are constructed from Bose symmetric sums of products of single particle wave functions in which each final state and initial state ^{4}He and d nuclear wave function possesses Bloch symmetry (associated with IBS's).

Then, for the purpose of establishing a bound for R, equation (10) can be used, in the limit that the bulk region remains in its GS (so that it does not contribute to R, and the approximate variational solution, associated with equations (12)-(18) can be used), and the contributions from the nuclear region can be assumed to involve initial and final IBS's that have vanishing wave-vector. Again for the purpose of deriving a lower bound for R, a one-dimensional model of the (many-body) overlap expression in the nuclear regions has been used [24]). Here, the CM distribution of the initial state nuclear wave function contribution (describing two potentially overlapping d's that asymptotically approach lattice dimension) is described using a Wannier state that mimics the behavior of a wave-packet, possessing the characteristic dimensions of a deuterium-like optical phonon. In particular, this Wannier state is approximated using the ground-state wave function of a 1-dimensional parabolic well with zero-point energy E_o=0.029.5 eV, possessing a characteristic dimension $a_{har} = \hbar / \sqrt{E_o M_D} = 0.5 a_e = 0.2646$ Angstroms,

$$\Phi_W(r) = \left[\frac{2}{\pi a^2}\right]^{3/4} e^{-\left(E_o M_D / 2\hbar^2\right)^2} = \left[\frac{2}{\pi a^2}\right]^{3/4} e^{-\left(\frac{r^2}{a_{har}^2}\right)}, \tag{19}$$

while the final state wave function is a minimal uncertainty wave packet Φ_{nuc} that has the characteristic dimension of a ^{4}He nucleus:

$$\Phi_{nuc}(r)=\left[\frac{3}{2\pi a_{nuc}^2}\right]^{3/4} e^{-\left(\frac{3r^2}{4a_{nuc}^2}\right)}, \tag{20}$$

where $a_{nuc} = 2 \times 10^{-13}$ cm approximately equals the radius of a ^{4}He nucleus. Previously [24], the 1-dimensional model associated with equations (19) and (20) has been used to evaluate the many-body nuclear overlap expression O_{nux}, defined in equation (11)

$$O_{nuc}=\left(\frac{16}{3}\right)^{3/4}\left(\frac{\mathrm{V_{nuc}}}{\mathrm{V_{har}}}\right)^{1/2}\times\left(1+\frac{4a_{nuc}^2}{3a_{har}^2}\right)^{-1}\approx\left(\frac{16}{3}\right)^{3/4}\left(\frac{\mathrm{V_{nuc}}}{\mathrm{V_{har}}}\right)^{1/2}, \tag{21}$$

where $V_{nuc}=(4\pi/3)a_{nuc}^3$ and $V_{har}=(4\pi/3)a_{har}^3$, and the error (which involves terms of order

$$\left(\frac{V_{nuc}}{V_{har}}\right)^{1/2}\frac{a_{nuc}^2}{a_{har}^2}\sim\left(\frac{V_{nuc}}{V_{har}}\right)^{1/2}\times 10^{-8}$$

and higher) associated with the last approximate equality is negligible. By substituting equation (21) into equations (10) and (11), it follows that

$$R=\left(16\!\!\diagup\!\!3\right)^{3/2}\left[\frac{2\pi\left(\Delta mc^2\right)^2}{\hbar}\right]\left[\frac{V_{nuc}}{V_{har}}\right]\rho_f(0)c_D^2c_{He}, \tag{22}$$

where $\rho_f(0)=1/\hbar\omega_{nuc}=4a_{nuc}^2M_D/3\hbar^2=0.773/\mathrm{MeV}$ is the final density of states (evaluated at the initial energy~0) associated with a harmonic oscillator (possessing angular frequency ω_{nuc}) that is consistent with the minimal uncertainty wave packet wave function, given in equation (20), and c_D and c_{He}, respectively, are the concentrations of deuterons that are initially in IBS's and ^{4}He nuclei that occupy IBS's after the reaction. In Chubb and Chubb, [24], by comparing the value of the power density $P=\left(\Delta mc^2\times R\right)\!/V_{cell}$, associated with equation (22), with a representative value [32] P=600 W/cm^3 that was observed in 1989, a relationship between c_D and c_{He} can be found:

$$c_D=\frac{4.7\times 10^{-9}}{c_{He}^{1/2}}. \tag{23}$$

and it was suggested that this last equality implies a lower bound (c_{LB}) occurs when $c_D=c_{LB}=4.7\times10^{-9}$. (Note the miss-print in [24], where it is stated that $c_D=4.3\times10^{-11}/c_{He}^{1/2}$.) And it was suggested that a lower bound for A more plausible bound occurs when $c_{He}=0.5\,c_D$, which occurs when each pair of d's that occupies an ion band state immediately becomes an ion band state ^{4}He nucleus. This last situation leads to $c_{LB}=3.5\times10^{-6}$, which is consistent with the value $N_{cell}\approx10^7$ that is appropriate when the Fermi Golden Rule applies.

5. Conclusion

In 1989, when FP made their initial cold fusion announcement, a firestorm of controversy erupted. With time, experimental confirmation of their observations not only occurred, reasons for the difficulties that

others had initially in reproducing their excess heat results are now more fully understood. An important source of confusion is that the fusion process that FP found is aneutronic and does not involve any high-energy particle emission. Instead, their heat is the result of a $d+d \rightarrow {}^4He$ reaction in which energy is released at levels that are commensurate with the amounts that are predicted by the difference in masses between the initial and final states. A logical rationale, based on a generalization of conventional solid state physics energy band theory, to situations involving finite lattices, can be used to explain the effect. The paper summarizes the underlying argument.

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