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CONTEXT FOR UNDERSTANDING WHY PARTICULAR NANO-SCALE CRYSTALS TURN-ON FASTER AND OTHER LENR EFFECTS

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Two persistent questions have been: 1. Why is it often necessary to wait for a finite period of time before the Excess Heat effect is observed after palladium (Pd) has been sufficiently loaded with deuterium (D), that the near full-loading condition (PdD_x, $0.85 \sim< x \rightarrow 1$) that is required for Excess Heat, has been achieved? 2. Is it possible to identify physical properties of the materials and/or crystals that are used that might be playing a role in the interval of time associated with this phenomenon? Recently, I generalized conventional energy band theory to address both questions. The new theory can explain these experimental results but will be ignored by most scientists. I suggest that this is expected: The context of energy band and Ion Band State (IBS) theory is very different from the context of hot fusion theory. Even within the Low Energy Nuclear Reactions (LENR) field, hidden, simplifying assumptions exist, which implicitly reflect biases associated with the context of hot fusion. A typical example is the idea that a single, particular form of reaction or environment can explain all LENR phenomena. As opposed to such a picture, involving a single "nuclear active environment" ("NAE"), the context of IBS theory and many-body physics suggests a more realistic and useful description of LENR involves a multiplicity of "nuclear active environments" (NAE's).

1 Introduction

Context can profoundly affect discourse and debate. Facts taken out of context can significantly misrepresent opinions or statements. Also, incorrect assumptions, resulting from context, can result in false conclusions. Thus, context can profoundly affect communication: For example, if a man yells "fire" or a fire alarm goes off in a crowded movie theatre, considerably greater harm can result, through potential panic, than if the same thing happens in a movie theatre containing a small number of people.

Over the years, Ion Band State (IBS) theory papers have focused on particular effects but have not included a complete description of the limitations and applicability of the theory. Thus, qualitative language, involving quasi-particles (for example) and other terminology has been used; while, in later discussions of the theory, a highly mathematical formulation was presented that many readers found difficult to follow. A useful context for understanding the Ion Band State (IBS) theory of Low Energy Nuclear Reactions (LENR) and its relationship to other theories or effects involving either hot fusion or LENR has not appeared. In particular, despite the apparent successes of the IBS theory, not only has the theory failed to be accepted, it has provoked unusual responses, including inaccurate statements, in separate Editorial comments in Nature magazine[1] and one of the ICCF conference proceedings[2,3]. These responses have a plausible explanation: IBS theory follows from a known context[4-6] (hydrogen in metals) that should apply to Cold Fusion (CF) but is inconsistent with hot fusion.

As the theory has evolved, more general ideas[7-9] have justified the underlying physics. Despite the fact that to date, no unifying theme or context for understanding the IBS theory in CF has appeared, the more general ideas relate to an important, unifying idea: The problem of relating crystal size to transport phenomena involving charged or neutral particles in finite lattices[10]. In particular, transport phenomena, in general, can become quite complicated in finite solids. But partial periodic symmetry can be used to identify a hierarchy of processes, in which all of the particles located in some "periodically-ordered" region, or some subset of it, can "move" coherently in a perfectly rigid manner (similar to the rigid, lattice recoil, in the Mossbauer effect) that preserves the separation between each particle with the remaining particles. These effects are the basis of a known phenomenon (an Umklapp process) that occurs in phonon scattering and electrical conductivity. In infinitely-repeating lattices, this process is described by a resonant effect, in which momentum is not conserved between "quasi-particles." Instead, the momentum is transferred to the lattice elastically. But momentum conservation requires that quantitative bounds exist for the amounts of momentum that can be transferred to a surface or interface (and vice-versa) through these kinds of processes. Traditionally, in models in which the lattice is infinitely-repeating and periodic, these bounds have been poorly defined. In finite solids, at low, but finite temperature T, precise, size-dependent bounds can be identified. In larger crystals, collisions with phonons tend to reduce the magnitudes of these effects. In smaller crystals (or in optical lattices[11]), this is not the case. In the case of palladium-deuteride (PdD), the effects can be quite large and can lead to coherent forms of interaction[12] and potentially LENR.

Initial estimates of the magnitude of the effects suggest a particular time scale for triggering the coherence that can be related to the incubation time[13] associated with CF. But, as in the past, this material was not introduced within the context, of a more complete theory[10,12]. The present paper includes a more detailed description, involving the context of the more complete theory[10,12].

This material, which is presented in the next section, provides a useful context for understanding the importance of the complete theory and its application in problems involving LENR. It includes a discussion of some of the earlier motivating work that led to the theory and material that provides a context for generalizing earlier results to more general problems involving LENR. The next and final section summarizes how the more complete theory can explain triggering in $d+d\rightarrow{}^4He$ in finite size PdD crystals.

2 Towards an Understanding of an Appropriate Context for LENR

2.1 Role of Context in Lack of Acceptance of Successes of IBS Theory

Beginning with ICCF1[2], we predicted[2,14] that by occupying IBS's, deuterons (d's) could initiate CF , without creating high energy particles, in a particular limit, involving "high-loading" (i.e., x→1 in PdD_x) in PdD. Here, IBS refers to a state that can be occupied by a deuterium nucleus (a "d"), in which the d effectively begins to behave in a wave-like fashion, similar to the way that an electron behaves in a periodically ordered solid; i.e., as a wave-like, "quasi-particle." In reality, this picture is a simplified description of the many-body physics, where the underlying effects occur in particular matrix elements associated with particular forms of overlap and rates of reaction. However, through this interpretation (involving quasi-particles), we suggested a number of effects, associated with the particular limit of full-loading, that can be used to justify a number of observed effects,[14] follow from very general features of the underlying physics. In particular, the physics of the d IBS limit requires that in Pons and Fleischmann (PF) experiments: 1. ^{4}He should be the primary product; 2. This product and heat should be the dominant phenomena[14,15]; 3. The reaction should not create high energy particles; 4. Neutrons and tritium can be present but in amounts that should not account for the heat and should be negligible in comparison to the amounts of ^{4}He; 5. That periodic order should be required on some time-scale commensurate with initiating the effect, and 6. High-loading should be required[14,15]. We also thought hard x-rays could be emitted[14] (during ICCF1) through the process that dissipates the heat.

Six months later[15], we suggested an alternative form of heat dissipation: That the lowest energy processes should occur through small fluctuations in D-loading that should approximately preserve periodic order inside a PdD host, the ^{4}He should occupy IBS's in the interior of the host, and that heating should take place in regions near the surface. As a consequence, based on a single physical picture (involving small fluctuations in loading in PdD), we suggested that the ^{4}He accounts for the heat and should be seen predominantly either outside heat-producing electrodes or in surface regions, near the boundaries of the electrodes. We made these predictions[18] in 1990 before experimental evidence was publicly disclosed (in 1991) that high-loading in PF experiments apparently was required[2,16] and the initial observation[17] that a correlation appeared to exist between Excess Heat and residual amounts of ^{4}He found outside heat-producing electrodes.

Two obvious limitations of the initial picture were: 1. It requires a particular kind of state (a quasi-particle band state), known to be useful in describing the behavior of electrons, but whether or not this state in an ionic form would be appropriate for describing CF effects as well as the behavior of d's in the limit of full-loading in PdD was not clear; and 2. Even in the case of electron transport, the quasi-particle energy band picture is approximate and conventionally applies (in metals, where transport phenomena have been most widely studied) only over large distances and when the externally applied fields vary sufficiently slowly. It was not at all obvious, within this context, that the associated picture could apply in a problem involving d+d fusion, where large changes in external fields could be required over short distances.

An important goal of the more complete theory[10,12] was to address both of these limitations from the outset. In order to accomplish this, a mathematically rigorous formalism, based on a generalized form of multiple scattering was developed[7], that could apply in finite lattices, was derived that potentially can also explain why high energy particles are not required in CF reactions. This formalism provided a way to generalize conventional band theory to cases involving finite lattices.

Within this context, it was possible to generalize conventional band theory by requiring that it apply to the ground state (GS) and lowest lying excitations and that the GS have minimal coupling to outside processes. Then, the lowest energy excitations of a solid, by construction, are required to conserve charge in some finite volume of the solid and are required to be unaffected by a symmetry: rigid translations (Umklapp processes) that preserve the separation between any two particles within this region[10,12,13].

We have made other predictions that have not been tested: 1. That when ^{4}He is externally introduced into the surface region and the region immediately outside heat-producing materials, it might catalyze the d+d→^{4}He reactions through a form of Bose-induced stimulation, similar to stimulated light emission in lasers[20]; and 2.That the observed anomaly (associated with the substitution of PdD for PdH) in the value of superconducting critical temperature T_c (in which T_c is higher in the case of PdD) might be the result of "Cold Fusion" at low temperature[21].

Because in the initial announcements, PF suggested that Excess Heat was the result of a colder version of conventional fusion, ideas, even tangentially related to cooperative forms of reaction, were entirely ignored. In an entirely unconventional and unjust manner, David Lindley[1] explicitly criticized these ideas and our theory almost a year after he received our first paper[22], without explicitly referring to our work, through his derisive comments[1] (about Bloch and Wannier states, and Bose Condensates): "[A] broad category of cold fusion theories rested on more sophisticated uses of collective effects [in solids]……..

"These theories had the special attraction that *they could easily be decorated with the jargon*, at once forbidding and enticing, of solid-state physics: Bose-condensates, Bloch states, Wannier functions… *like the Paris fashions, they outface mockery…*

"Nevertheless they were all wrong, and for a ..straightforward reason. The fusion rate for two deuterons is calculated from their two wavefunctions, multiplied by the nuclear interaction rate. The latter is a very short range force, only at separations of a few nuclear radii is the nuclear reaction rate significant. The only important contribution to the fusion rate, therefore, comes from the product of the wavefunctions when the deuterons are very close. But the wavefunctions in the Bose-condensed state are calculated explicitly by ignoring the nuclear interactions; they are valid everywhere except at close range."[1]

During ICCF2[2], Giuliano Preparata also criticized our theory[2,3] because it appeared to ignore the key problem (involving the Coulomb barrier) that seemed to be relevant in the CF problem. In fact, both sets of comments reflected biases, associated with conventional fusion. However, as opposed to Lindley's approach, which involved first ignoring the relevant science in our paper, not publishing the material, and then criticizing its ideas (based on incorrect information about the relevant physics), without appropriately referencing the material, not only did Giuliano Preparata allow our ideas to be published, but he actively participated in a useful scientific debate about their relevance.

Lindley's comments had some value. He pointed out (as in conventional fusion) close proximity between d's, at a single location, is required for a nuclear reaction to occur, and effects of electromagnetism (EM) can be treated as being static, relative to the dynamical effects involving the nuclear forces (NF's). This picture applies to conventional situations involving higher energy incident particles in nuclear reactions, and especially in hot fusion, where deuterons have a sufficiently large incident kinetic energy. Then , the time- and length- scales involving EM and NF's are so different that the total wave function Ψ can be factored into the product of separate components Φ_{nuc} and Φ_{em} (through the d-d separation variable r) :

$$\Psi=\Phi_{nuc}(r)\Phi_{em}(r). \qquad (1)$$

In ordinary $d+d\rightarrow{}^4He+\gamma$, in fact, at all times, the dependence of the coupling to the electromagnetic field must be included[23]. Although this fact has been known since the early 1970's, it does not appear in conventional fusion literature because the $d+d\rightarrow{}^4He+\gamma$ occurs at a rate that is $\sim10^7$ times slower than the comparable rates associated with the dominant ($d+d\rightarrow{}^3H+p$ and $d+d\rightarrow{}^3He+n$) reactions. On the other hand, the reverse reaction, ${}^4He+\gamma\rightarrow d+d$ has been studied in detail. Here, it is known in fact, as opposed to the reaction involving the simple form, associated with Eq. 1, a comparable factorization between NF and EM wave functions is not possible because the associated dynamics requires detailed information[23] about the coupling of the EM interaction with the NF.

Lindley misquoted this as well as a number of additional facts, including the nature of the $d+d\rightarrow{}^4He$ reaction, which he had not investigated, and the fact that d's have unit spin. Also, at the time, important information about the nature of products was not known. With hindsight, his comments illustrate a misunderstanding of fundamental aspects of many-body physics. In particular, although in 1989, Bose Einstein Condensates (BEC's) had only been observed in natural processes in cryogenic environments, involving near absolute zero T in helium, non-cryogenic procedures involving laser-cooling were being developed for creating BEC's. Beginning in 1995, these procedures made it possible to dynamically create BEC's. Since that time, not only has it become possible to create, manipulate, and alter BEC's, using lasers but to artificially stimulate phase transitions, in which states involving an initial configuration of localized bosonic atoms (that remain confined in regions of space, defined by particular lattice sites in an optical lattice) into delocalized (coherent) states in which the bosonic atoms exhibit the kinds of wave-like behavior, that we suggested might be relevant, are produced routinely.

2.2 A Meaningful Context for LENR based on Broken Gauge Symmetry

Although Lindley was conceptually wrong, his use of Eq. 1 illustrates an important source of confusion: Eq. 1 is based on a number of assumptions involving length and time scale. In particular, the associated picture assumes that because nuclear reactions are initiated, with high energy, initially, the effects of EM can be ignored. In hot fusion, this makes sense since in hot fusion, a form of perfect "SU2 symmetry" can apply, in which it is never possible to distinguish between protons and neutrons. In the normal nuclear physics scenario, then, to have protons and neutrons close enough together for reaction to occur, it is assumed they occupy a state involving asymptotically free nucleons, in which effects of EM can ge ignored. as Giuliano Preparata emphasized.

In fact, when additional symmetries are present, this picture need not apply. At non-infinite temperature and energy, residual EM interactions are present that break SU2 symmetry. In all situations, the process of lowering the energy requires loss of symmetry. This occurs because of a general requirement: The GS, by definition, to be stable, must have the smallest overlap with outside processes. When many particles are present, however, as opposed to a gradual reduction in symmetry, involving de-excitation between states, near the asymptotically free state (assumed as the intial state in nuclear physics), an entirely different situation can occur, provided the overlap process involves changes in momentum and energy, involving the EM interaction. In particular, as opposed to de-exciting an initial state, involving asymptotically free particles, an initial state involving potential nucleon overlap can form through an approximate symmetry, and the de-excitation process can result from an instability associated with the symmetry.

Within this alternative context, as opposed to nuclear reaction being initiated from an extremely excited state, involving a small number of particles, a combined motion of many particles, at or near the GS configuration, can take place and lead to nuclear interaction. From this near GS configuration, as opposed to forms of interaction that couple the highest possible states of excitation with an effectively asymptotically free state, the de-excitation process can involve many particles that all have effectively the same energy and momentum, in a configuration in which all particles actually have negligibly small kinetic energy. An important symmetry that can cause this is associated with the peculiar limit (involving the kind of rigid-body, Mossbauer-like, Umklapp processes, alluded to above) in which many particles, at once, move rigidly, in such a way that the separation between any two particles remains the same. This can be accomplished through a second observation, made by Preparata: That the zero of momentum can be altered, dramatically, by a classical motion, involving many particles moving in a particular way. An important point that Preparata did not fully appreciate, however, is that it is never possible, a priori, to constrain a collection of particles within a particular volume, in such a way that the locations of the particles can be identified. Because the velocity of any particular, rigidly moving configuration, relative to the velocity of a second rigidly moving configuration, can be continuously varied, a large degeneracy exists, in principle, associated with many, closely-related, rigidly moving configurations.

In fact, in the absence of charge accumulation at the boundaries of a solid, these different configurations are related, in principle, to each other through a (trivial) but continuously varying change in a particular parameter (the center-of-mass momentum) that can be related to the choice of gauge[12], associated with the vector potential. As a consequence, the associated symmetry is referred to as gauge symmetry. In the limit in which this form of symmetry becomes dominant, asymptotically, in a sufficiently large solid, it is possible to require that far from the boundaries of the solid, effectively, in the evaluation of any relevant matrix element (associated with a particular many-body process), Eq. 1 remain valid for any configuration involving nucleons, provided no change occurs in the relative separation coordinate (r) between the center-of-mass (CM) coordinates of different charged particles (associated with the behavior of $\Phi_{EM}(r\ )$) in regions located far from potential overlap with NF's; while in regions where the relative separation in CM coordinates overlap with NF's, changes are allowed to take place, provided the resulting changes in momentum are all transferred to a total change in the CM momentum of the solid, through an Umklapp process. From such a starting point, Preparata's idea that many particles can move at once can be generalized: Instead of one configuration moving classically, with a single momentum, all possible configurations, in which each configuration is related to the others by a fixed difference in momentum, can be allowed to take place.

In all relevant interactions, all momentum from a potential LENR can be transferred instantly[12] to the CM without altering the relative energy or momentum in interior regions where the EM interaction is dominant. Formally, this requires that energy and momentum are conserved, but how this occurs is ambiguous since it is not possible to determine the locations of the charged particles within a particular volume. Within the constraints of this limit, the form of separable wave function, involving Eq. 1, can be generalized: Instead of particular pairs of d's (as we initially suggested), associated with conventional fusion, at far separation (through $\Phi_{EM}(r\ )$, where r is large, relative to NF overlap) or at near separation (where Φ_{nuc} (r) applies, at locations where r has overlap with NF's), each function $\Phi_{EM}(r)$ or $\Phi_{nuc}(r\ )$) can be interpreted as involving a collection of charged and neutral nucleons. The requirement that changes in the nuclear coordinates only alter the CM momentum, in turn, and not lead to changes in the relative separations between charged particles, in the interior (bulk-like regions[10,12]) can lead to particular selection rules. In particular, in the early stages of the development of the IBS theory, we suggested an approximate selection rule: That the dominant d-d reactions involve changes in wave function through variations in nuclear coordinates (and potential nuclear reactions) not alter the wave function $\Phi_{em}(r\,)$ at locations that are asymptotically far from the location of any possible NF overlap. In fact, in the more rigorous formulation, all possible forms of overlap become possible, and the comparable constraints need not apply except either near the GS or when the system is prepared appropriately. However, a generalized result also is appropriate: Eq. 1 still applies in the most coherent forms of reaction, provided the definitions of $\Phi_{nuc}(r\,)$ and $\Phi_{EM}(r\,)$ are generalized: As opposed to referring to the wave functions describing proton-neutron (p-n) pairs, in any particular reaction rate, the associated wave functions can be interpreted as describing the CM motion of collections of p-n pairs, or p-n pairs coupled to p's and/or n's, or, more generally, of collections of charged particles (p-n pairs, p-n pairs with p's or n's, or p-n pairs, with p's and/or n's and electrons).

An important point is that although larger clusters of charged particles (in the relevant portions of a particular matrix element) can be viewed as generalized forms of quasi-particles, need not be forbidden, with increasing size, possible effects involving broken symmetry (through alternative forms of overlap in other matrix elements) become more likely and: The most coherent coupling involves simpler configurations, but these can cause greater degeneracy and greater instability. The key point is that the states that have the greatest overlap with the GS are required to not alter the relative coordinates between charged particles or clusters of particles in the regions (associated with EM interaction) far from the locations of nucleon overlap and NF interaction. From earlier arguments[24] , this more general context can be used to generalize the earlier selection rule[14,15,22]. The lowest energy excitations require that when $\Phi_{em}(r\,)$ is a boson (i.e., its total spin is an integer multiple of $\hbar$), $\Phi_{nuc}(r\,)$ is also a boson; and when $\Phi_{em}(r\,)$ is a fermion (i.e., when its total spin is an odd multiple of $\hbar/2$), $\Phi_{nuc}(r_{nuc})$ is a fermion.

An important point is that this last set of rules is approximate and is only required to apply in crystals that are sufficiently large or when other factors (for example, through changes in the fluxes of particles into and away from the solid, or through external fields) might require that these rules apply. An unfortunate result of the history of CF and LENR, and in the initial context of hot fusion, is that it has been frequently assumed that a single set of conditions, associated with what has been called a "nuclear active environment"[25] (NAE) has been believed to be responsible for LENR. Gauge symmetry, and broken or approximately broken gauge symmetry imply a considerably richer, different scenario. To the degree that particular gauge symmetries (for example, those associated with an applied electric field) can be important, specific triggering phenomena can be important. In other situations (for example, those involving a magnetic field, or varying flux of charged and/or neutral particles), depending upon the potential overlap between possibly degenerate states with external fields, many different effects can take place. Magnetic coupling, in particular, can alter potential channels for nuclear reaction in profoundly different ways involving "bosonic" or "fermionic" coupling. Also, it certainly is not required that Eq. 1 apply either to pairs of deuterons or charged (fermionic or bosonic) "clusters" of particles, or that when it does, the lifetime of the associated state is sufficiently long that appreciable overlap with NF processes take place. In fact, whether or not a particular kind of reaction will take place involves a complicated reaction rate expression, based on a true many-body configuration. In particular limits, loss of symmetry and gauge symmetry (through broken gauge symmetry) can become important. But this certainly is not a requirement for LENR.

3 Why Particular Nano-Scale Crystals Turn-On Faster

In analyzing the possibility of transferring momentum rigidly from a nuclear reaction to the CM of a finite crystal lattice, without altering the energy of any of the particles in the lattice, I realized that a similar effect could be used to explain how an applied electric field $\vec{E}$, potentially, could shift the momentum of many charged particles, at once, rigidly, without changing the relative separations between any of the particles. Limits of the associated picture can be quantified through a generalized form of multiple scattering[7] that I developed for the CF reaction problem. Applied to the $\vec{E}$-field problem, the argument generalizes the conventional Bloch (wave function), quasi-particle theory of electron conduction[10,12], based on energy band theory in infinitely-repeating, periodic lattices, to situations involving finite lattices involving charged particles (either electrons or hydrogen nuclei). In the new theory: 1. I generalized Bloch's theorem, to a many-body form; 2. The vague notion of transport phenomena involving quasi-particles is re-defined rigorously, through changes in the zeroes of energy for each set of indistinguishable particles; and 3. Transport occurs through a change in the physical momentum involving each energy band state, which is a possible zero of energy, relative to the classical turning point of the kinetic energy. Here, reaction rates establish the relative time-scales of potential processes. The GS is required to have minimal overlap with states that are degenerate with it in the limit that far from the boundaries of the solid, a lattice exists, in which the net flux of particles into and away from the lattice vanishes. Since in the absence of accumulation of charge at the boundary, there is no way to distinguish the zero of energy of a particular many-body state from a second many-body state that is identical to it, except that it is moving, relative to it at a constant uniform velocity, a huge number of states can be degenerate with the GS as a result of implicit forms of invariance with respect to Galilean transformations (i.e., through Umklapp processes) that preserve particle-particle separation. As a consequence, Umklapp processes are defined uniquely and can provide large amounts of momentum coherently to the center-of-mass (CM).

During the prolonged electrolysis of D_2O by PdD a situation that mimics this limit can take place[9,10,12,27] as a result of small fluctuations in loading ($\delta = \pm 0.03\%$) in finite $PdD_{1+\delta}$ lattices. In finite $PdD_{1+\delta}$ crystals, the associated loading-induced motion of Pd nuclei that results from these fluctuations has a small deuteron component that involves IBS occupation since each fluctuation extends throughout the solid and carries charge. In large lattices, the IBS's do not conduct appreciable ion charge because for all values of the wave-vector k, their energy ε is the same:

$$\varepsilon = \varepsilon(k) = \varepsilon(0) \qquad (2)$$

When Eq. 2 holds approximately, the collisions that prevent coherent Umklapp processes are stifled, and the IBS effectively mimics the kind of state that electrons occupy in an insulator. From this starting point, because collisions are stifled, it becomes possible for a phenomenon similar to Zener/Electronic breakdown[25] to take place, in which ions (as opposed to electrons) tunnel into a higher, conducting energy band state (an IBS), after a critical period of time. In this form of Zener/Ionic breakdown, the tunneling time depends on crystal size. Crystals that have characteristic dimensions smaller than ~6 nm, which have tunneling times~microseconds, either are not capable of providing enough momentum to create heat (through $d+d \rightarrow {}^4He$) or conduct so rapidly that collisions occur. Crystals with dimensions~60nm will create heat and load rapidly (~3 ms). But tunneling time scales by 1000 as the characteristic dimension increases by a factor of 10, and crystals with more than ~60 microns have tunneling times that are longer than a month. This suggests that the incubation times, observed in the experiments are the result of crystal size and (as suggested by Arata's results[26,27]) that nano-scale crystals turn-on considerably faster than micro-scale crystals.

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