Quantum Mechanics of "Cold" and "Not-so-cold" Fusion

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Abstract

Cooperative ionic fluctuations, which become energetically favorable during the overcharging of a sufficiently ordered, stoichiometric Pd-D lattice, provide a means for an entirely new form of nuclear interaction, "cold" or "solid state" fusion. As a consequence, 1) nucleons separated by macroscopic distances *in a classical sense* may interact in a nuclear fashion *quantum mechanically*, and 2) nuclear fusion may occur in which unfamiliar products are released. The evolution of such an ionic fluctuation, which we have named a Bose Bloch Condensate (BBC), becomes favorable as the concentrations of D and Pd become comparable because of large energy costs from lattice strain at individual lattice sites that result from coulombic repulsion associated with the occupation of a site by more than one D. These strain energy costs are removed through the evolution of long-ranged, periodic, ionic fluctuations in which equal (though small) amounts of excess charge are distributed uniformly to unit cells throughout the crystal. We provide the underlying quantum mechanical theory that governs both the evolution of these fluctuations and the associated selection rules of the resulting nuclear interactions. We also use a critical element of this theory (associated with the electrostatically induced changes in volume that accompany the binding of D^+ ions to an external environment) to explain how it is possible to initiate the kinds of low temperature fusion reactions that apparently have been seen in the recent Cluster Impact Fusion experiments performed by Beuhler, Friedlander, and Friedman.

Introduction

It has not been generally recognized that at the current time there is an evolving taxonomy of fusion processes. The first and best known form is "hot fusion", which is initiated from free space collisions of deuterons at high temperature. The two remaining forms were discovered during the last year. In both forms, fusion seems to be initiated at considerably lower temperature. These recently discovered processes are "cold fusion" as observed by Fleischmann and Pons[1], and "not-so-cold" fusion as observed in ion cluster impact experiments by Beuhler, Friedlander and Friedman[2]. In cold fusion, heat is produced without proton or neutron generation, whereas in not-so-cold fusion there is a release of neutrons and protons, as in conventional hot plasma fusion, but the process occurs at deuteron bombardment energies well below those known to be effective in D-D fusion-inducing collisions.

Both cold and not-so-cold fusion are manifestations of the quantum wave character of particles at low energy. The behavior of a particle as it undergoes collisions at low energies is determined both by the intrinsic properties of the particle and by the environment in which the particle resides. In the language of physics and chemistry, the wave function of a particle is determined by the interaction possibilities and by the boundary conditions applied. In a semantic extrapolation, one could say that the structure of a particle is affected by the boundary conditions it sees. Disregarding the semantics, quantum mechanics provides procedures for calculating particle behavior; namely, one calculates the wave function in accordance with the boundary conditions and pertinent interactions, and one calculates reaction rates using overlap integrals in accord with the Fermi Golden Rule or its equivalent.

Once it is recognized that the boundary conditions associated with bound deuterons may profoundly affect the quantum mechanical dynamics of colliding deuterons, it is possible to understand 1) how it is possible (contrary to conventional expectation) to initiate fusion in low temperature environments, and 2) that there is a relationship between the two lower temperature forms of fusion. Because Cluster Impact Fusion is highly reproducible while cold fusion is difficult to reproduce, the fact

that such a relationship can be explained quantum mechanically is significant.

The key difference between free space, unbound deuterons and deuterons that are bound to an attractive potential is that unbound deuterons may occupy any region of space with an appreciable probability, while the probability of finding a bound deuteron in a region of space beyond the classical turning point of its motion is exponentially small. Thus, when the active reactants in a fusion process obey the boundary conditions associated with bound deuterons, the potential for overlap during collisional processes becomes very different. As a consequence, if the active reactants are bound, many of our preconceived notions about fusion (which are based on the boundary conditions associated with unbound deuterons) do not apply.

Cold fusion is more complicated than ion cluster impact fusion, but both fusion processes depend on the existence of deuteron wave functions broadened to ~ 0.2 A by zero point motion. This wave function broadening is a consequence of electrostatic interaction between bound D^+ ions and the electrostatic potential provided by the other atoms and electrons of the larger structure that bind the D^+ ions to a particular region of space.

Quantum Mechanics of "Not-so-cold" Fusion

Let us first consider the cluster ion impact experiments. In the cluster impact studies D_2O ion clusters are accelerated onto a Ti target containing deuterium. The cluster ions are mass filtered so as to remove any light ion clusters or "naked" D^+ ions present in the beam prior to acceleration. (Here, a "naked" D^+ ion refers to a singly charged ion which is not bound to a cluster.) Control studies have shown that no high energy light ions contaminate the filtered heavy ion beam. The studies are carried out at ion impact velocities that correspond to D^+ kinetic energies relative to the target frame of ~100 eV. Fusion reactions are observed[2] at a rate that exceeds conventional expectation (based on the free space picture associated with the Gamow theory of a point particle electrostatic barrier) by more than a factor of 10^{10} . Fusion is not observed when the target contains H instead of D. Beuhler et al measured the fusion rate for impacting clusters over a wide range of cluster sizes having a fixed 300-KeV total energy. They found beginning at low mass that the fusion rate increases with cluster mass, going through a maximum near $D^+(D_2O)_{200}$. For this case the kinetic energy of the impacting D^+ ions in the target frame is 150 eV, far below the value at which a D^+ beam impact fusion would be expected based on Gamow theory.

It is clear from calculations given below that Gamow theory does not apply when the zero point motion broadening of the wave function is included in the target D that results from binding of the target D to the Ti host. To our knowledge, it is an open question what the actual value is of the fusion rate of a beam of D^+ incident on a TiD_2 target at these energies. Presumably, this rate is considerably smaller than when the incident D resides either within a cluster or bound to a single O atom or to an OD because when the D is bound to any of these polyatomic entities, its wave function is also broadened as a consequence of the binding that results from its interaction with its environment. Even for the case in which the incident D are "naked" (i.e., not bound to a cluster as they are in these Cluster Impact Fusion Experiments), for a wide range of energies Gamow theory simply does not apply when the target D is bound (as shown below), and the exponentially small value (associated with conventional wisdom) for the fusion rate at the energies associated with the average D energy (~100's of eV) in these collisions does not apply.

Because the effect of wave function broadening in the target D dramatically expands the "effective", electrostatic volume of each D by many orders of magnitude relative to its "point-like", free space size, even a crude calculation can be used to demonstrate how this wave function broadening effect may significantly alter the electrostatic barrier that inhibits fusion. Specifically, we may approximate the broadening effect by using for the target D wave function Φ^{target} the ground state wave function for a harmonic well, whose curvature is defined by the characteristic zero point motion R_{zp} (as determined by neutron scattering experiments) of D in TiD_2.

$$\Phi^{target}(R) = (2/(R_{zp}^2\pi))^{3/4} \exp(-R^2/R_{zp}^2) \qquad (1)$$

For the incident D wave function Φ^{inc} we may use a minimal uncertainty wave packet of characteristic size λ_{inc}, defined by the approximate variance of the deuteron wave function during the collision.

$$\Phi^{inc}(R) = (2/(\lambda_{inc}^2 \pi))^{3/4} \exp(-R^2/\lambda_{inc}^2) \qquad (2)$$

Depending upon the circumstances associated with the collisional process, λ_{inc} may take on a wide range of values. Since 80 percent of the momentum in each D_2O molecule is given to the oxygen atom, and the oxygen atom possesses 90 percent in each OD molecule, it is clear that as the cluster breaks up during the impact with the solid, transfer of energy and momentum from the O to the solid provides the dominant mechanism for slowing down the incident particles. In addition, as these momentum transfers occur, it is to be expected that significant interaction through changes in the vibrational modes of the D through bonding with the O will occur. Thus, we expect that the wave function broadening associated with O-D bonding and with changes in this bonding associated with interaction of the O with the solid will provide the dominant effects associated with the characteristic dimension λ_{inc}. The associated zero point motion is again on the order of 10^{-9} cm provided that the D remains bound to the O. If it becomes unbound, its characteristic dimension can vary considerably, with a lower bound corresponding to the situation in which the incident D has energy of ~100's eV. This case leads to the value $\lambda_{inc} \sim 10^{-10}$ cm.

Not surprisingly, when a realistic value of R_{zp} (~2 x 10^{-9} cm) is assumed, each deuteron is only "weakly" bound to a particular zero point volume of the lattice (it has a zero point energy of 10's of meV). The result of a first Born calculation of the shift $\Delta E^{(1)}$ in eigenvalue of each target deuteron that results through Coulombic interaction then is a "large", repulsive perturbation relative to both this electrostatic binding energy and to the binding energy of the deuteron to the entire crystal (given by ~ the heat of desorption ~ several eV). Thus, not only will the incident projectile unbind the target from its zero point volume, it will unbind the target completely from the lattice. Specifically,

$$\Delta E^{(1)} = e^2 \iint d^3R\, d^3R' \frac{\Phi^{target}(R)^2\, \Phi^{inv}(R')^2}{|R - R'|}$$

$$= e^2 (2/(\pi(R_{zp}^2 + \lambda_{inc}^2)))^{1/2}$$

$$\sim 30 \text{ eV} \qquad (3)$$

Then, the collision induces an electrostatic repulsive shift in the eigenvalue that is several hundred times larger than the zero point energy of the target, and about ten times larger than its total binding energy to the lattice. However, this shift in eigenvalue is 5 orders of magnitude less in absolute value than the accompanying attractive shift in eigenvalue that results from the strong interaction. The shift is also five orders of magnitude less than the comparable electrostatic shift that results when "point-sized" particles of nuclear dimension collide in this fashion. As a consequence, prior to and in the presence of the perturbation, the characteristic electrostatic and nuclear energies remain very different when the target D is initially bound, while this is not the case when the target and incident D are both unbound. Because these energy scales are so different, it becomes possible to write the "complete" wave function $\Phi = \Phi(r_n, r_p)$ (r_n and r_p respectively are the coordinates of the proton and neutron) for the target and incident D approximately in a Born-Oppenheimer separable form in which variations in the center of mass coordinate, $r_{cm} = (r_n + r_p)/2$, (which are associated with electrostatic interaction, as in the R and R' dependencies of Eqs. 1-3), are independent from the short-ranged variations in neutron-proton separation $r_{n\text{-}p} = r_n - r_p$ that are associated with the strong interaction.

$$\Phi = \Phi^{elect}(r_{cm})\, \Phi^{nuc}(r_{n\text{-}p})$$

Here, $\Phi^{elect}(r_{cm})$ is a slowly varying function, whose value is appreciable on the length scale of the electrostatic interaction, while $\Phi^{nuc}(r_{n\text{-}p})$ has appreciable value only on the length scale of the strong interaction. When this separability condition is imposed, it then follows that the first Born shifts in eigenvalue are extremely negative, indicating that fusion *may* occur. However, because the electrostatic perturbation is large on the scale of the initial energy (10's of meV) of the target D, the perturbation expansion must be viewed

as asymptotic at best, and coupling to higher order perturbations may alter the eigenvalue shift in a manner that would invalidate this conclusion.

On the other hand, it is also true that during the collision process, coupling to electrons (and other atoms through the electron coupling), could broaden the wave function further. Because there are wide possibilities associated with this effect, it is probable that perturbation theory may be applied. Then, it follows that fusion becomes permissible. In this manner, we see that as a consequence of broadening induced by the target, it becomes possible for a very different scenario to unfold in which fusion *may* occur. The additional broadening that results as a consequence of binding between the incident D with other atoms before and during the collision process probably plays a role in the resulting enhancement in fusion rate. Through even these crude arguments, we see that 1) cluster impact fusion follows as a consequence of wave functioning broadening due to binding effects associated with interaction between both the target and incident deuterons with their respective external environments, and 2) the effect should be sensitive to variations in cluster size. Thus the observation of cluster impact fusion and our explanation of the phenomenon provide a convincing demonstration of how the effect of wave function broadening may significantly alter the coulomb barrier to fusion.

Since the boundary conditions associated with cluster impact fusion and with colliding particles in free space are very different, it would be surprising if the Gamow theory (associated with free space collisions) has bearing on this new form of fusion. In fact, a crude application of the theory can be used to demonstrate that even for the case of a "naked" unbound deuteron incident on a target D, binding of the target to the Ti host may so significantly alter the resulting Coulomb barrier that in the majority of cases (i.e., when the incident D has an energy greater than ~70 eV), the underlying principle associated with the barrier concept (i.e., that "tunnelling" is required) breaks down. Specifically, when the incident D is sufficiently energetic so that the overlap of its wave function with the target wave function of Eq. 1 is sufficiently small, it follows that the repulsive Coulombic barrier V^{Coul} associated with the tunnelling problem may be evaluated in the limit in which the response of the target density to the presence of the incident deuteron is neglected. In this limit, the tunnelling probability T is given by

$$T = \exp(-2\lambda) \qquad , (4)$$

where

$$\lambda = \int_0^{r_{tp}} dR \left(\frac{(V^{Coul}(R) - E)2M_D}{\hbar} \right)^{1/2} \qquad , (5)$$

r_{tp} is the classical turning point (defined by $V^{Coul}(r_{tp}) = E$), E is the incident energy, $\hbar = h/(2\pi)$, where h is Planck's constant, and M_D is the mass of a deuteron. Also, because the response of the target to the incident D is neglected, $V^{Coul}(R)$ is the Coulombic potential that the incident D "experiences" due to the presence of the target D.

$$V^{Coul}(R) = e^2 \int \frac{d^3R' \Phi_{target}(R')^2}{|R - R'|} \qquad (6)$$

Using Eq. 1, it follows that

$$V^{Coul}(R) = e^2 (2/(R_{zp}^2\pi))^{3/2} \frac{1}{2\pi^2} \times \int d^3Q \int d^3R' \left\{ \exp(i(Q\cdot(R-R')) \times \exp(-2R'^2/R_{zp}^2) \right\} / Q^2$$

$$< (8/\pi)^{1/2} e^2 / R_{zp}$$

$$\sim 70 \text{ eV} \qquad .(7)$$

This last inequality means that there is no classical turning point whatsoever associated with Eq. 5 when the incident energy is greater than 70 eV. Thus, for E>70 eV, the fundamental idea associated with a tunnelling requirement (as in Eq. 4) breaks down since the forbidden region in which exponential decay of the wave function occurs is never involved in the collision process.

Quantum Mechanics of "Cold" Fusion

Zero point motion plays an important role in cold fusion, but its role is different than in cluster impact fusion. It causes a reduction in the electrostatic interaction energy associated with the transient multiple occupation of a lattice site. Multiple occupations arise quantum mechanically from self-interaction of identical bosons in a periodic lattice. A key aspect of this self-interaction is the approximate notion of periodicity. When periodicity prevails for a sufficiently long period of time, for each Bravais vector of the lattice R_n, the single particle wave functions ψ associated with the stable particles (with respect to the electrostatic interaction) obey Bloch's theorem,

$$\psi_{\mathbf{k}}(r+R_n) = \exp(ik\cdot R_n)\psi_{\mathbf{k}}(r) \quad . \quad (8)$$

Because the long-lived states obey Eq. 8, it follows that at an isolated location, the density is constructed from a superposition of states, formed from the eigenstates that obey Eq. 8. In this context, at any moment in time, at an individual lattice site the density must be viewed as a transitory entity, which oscillates in time. Of greater significance, when the many-body wave function is constructed from wave functions that obey Eq. 8, it follows that at any moment in time, there exists the possibility at a given site of fluctuations involving one, two,...N_B bosons (N_B is the number of bosons in the entire crystal), where the lifetime of this kind of fluctuation is determined by the interaction time associated with self-interaction.

The main effect of wave function broadening is a lengthening of the electrostatic lifetime (due to self-interaction) of the resulting multiple occupation virtual states. Because there exist a large set of self-interaction processes (each of which may be constructed self-consistently), in which Born-Oppenheimer separability applies as a consequence of large disparities in the energy, length and time scales between the perturbations associated with electrostatic and nuclear self-interaction, it follows that once states become occupied in which the scales of these interactions are sufficiently different, analogous to the evolution of the separability condition that arises in cluster impact fusion through wave function broadening, Born-Oppenheimer separability applies both prior to and in the presence of a well-prescribed perturbation.

The major distinction in the case of cold fusion is that the perturbation is always derived from self-interaction between bosons in which Born-Oppenheimer separability applies and is maintained. (When only those perturbations which preserve the separability between nuclear and electrostatic wave functions are included, the theory becomes self-consistent.) A necessary and sufficient condition which unambiguously preserves the condition of separability is that the wave function field associated with the single particle electrostatic interaction (from which the stable entities are constructed) must evolve in a manner that is independent of the more rapidly varying wave function fields associated with the nuclear interaction. This condition, once the fields are quantized, can only be maintained when the stable entity from which the field theory is formulated involves tightly bound proton-neutron pairs, which on the scale of electrostatic interaction behave as bosons. This result leads to the selection rule of cold fusion: *when the initial state is composed of tightly bound proton-neutron pairs, the final state is composed of tightly bound proton-neutron pairs.*

The distinction between the electrostatic and nuclear self-interactions is somewhat arbitrary. As long as there exists a well-defined set of perturbations, all of which are of sufficiently short length and time scale, and a second set of perturbations which are considerably longer in length and time scale, Born-Oppenheimer separability can be maintained. In fact, because, to an excellent approximation, the strong interaction remains invariant with respect to rigid displacements of the reactants and products, the strong interaction associated with a given multi-particle fluctuation is cyclic in the center of mass coordinate of the fluctuation. In practice, by expanding any of the relevant many-body interactions about the center of mass coordinate of all of the entities involved, it always becomes possible as a consequence to separate the self-interaction into two pieces, one of which is "slowly varying" and depends on the center of mass of the fluctuation, while the second is considerably more rapidly varying and does not depend on the center of mass. As the number of particles involved in the fluctuation increases, this kind of

separability procedure becomes artificial in the sense that there is no clear-cut difference in length scale. Provided, however, we restrict consideration to sufficiently simple forms of fluctuation, the ratio of the electrostatic lifetime (where this lifetime is associated with the slowly varying perturbation) to nuclear fluctuation time (associated with the rapidly varying portion of the perturbation) becomes sufficiently small that the wave function of the multi-particle fluctuation can always be written as a product of functions, in which one function is slowly varying and depends only on the center of mass coordinate of the fluctuation, while the remaining functions do not depend on the center of mass. This prescription provides a means of generalizing the Born-Oppenheimer separability of the many-particle fluctuation in a manner in which the kinds of perturbation theory arguments associated with cluster impact fusion can be applied to cold fusion.

Let us now consider the band theory of cold fusion[3-6]. The theory applies the quantum mechanics associated with the energy band theory of solids to D^+ ions in a periodic solid and examines the self-interactions implicit in the many body bosonic wave function that describes band state D^+ ions. The theory is a composite theory in the sense that it depends on a number of possibly controversial steps. These steps are:

* The occupation of band states by a macroscopic number of indistinguishable D^+ ions,

* the use of quantum mechanics and many-body theory to account for the associated quantum field behavior of the D^+ that occupy these band states,

* the effect of the environment on the structure of particles at low energy that are initially bound to a lattice, and the incorporation of this effect in the initial state band picture from which fusion commences,

* the relevance in this quantum field problem (as it relates to the nuclear fusion problem) of transient, cospatial multiple occupations of lattice sites by band-state D^+ ions (which are present in the initial state as a consequence of Bloch symmetry),

* the relevance to the fusion problem of a category of self-induced potentials associated with the short-range behavior of the field theory, each of which preserves Born-Oppenheimer separability, and the neglect of all other perturbations,

* the subsequent transfer of momentum to the environment from a model final state in which both the electrostatic and nuclear wave functions are of comparable dimension but are uncorrelated with respect to each other.

Each of these steps is in accordance with the laws of physics. It is not necessarily clear that the realization of the limit in which our theory would apply has been observed. However, even rudimentary calculations indicate important predictions of the theory seem to apply. These include the following: 1) it is necessary to achieve an over-potential condition prior to obtaining the anomalous heating effects in the electrolysis experiments, 2) in the case of Pd, the anomalous heating will occur very near the concentration $x=1$ in PdD_x, 3) there is a selection rule that is required by Born-Oppenheimer separability (as discussed above) and the nature of the interaction that mandates that in the primary cold fusion reactions, when the initial state involves only deuterons, the final state can only be formed from particles that consist of proton-neutron pairs. Thus, the theory predicts heat release without production of primary neutrons or protons. The possibility of the release of 23.8 MeV alpha particles is indicated, but a prediction of the number of alphas per joule of energy release requires a better understanding of the final step. Although there undoubtedly are refinements in the details of the theory that will be needed to understand all aspects of cold fusion, even in its initial (somewhat crude) form, the theory seems to provide a framework for an understanding of the cold fusion phenomenon.

Let us now summarize the band state D^+ cold fusion model. We can then discuss the individual statements making up the summary.

"Cold" Fusion in PdD_x at $X=1+\epsilon$

Injection of deuterium into metals containing a maximum loading of chemically

bonded D creates a population of band state deuterium ions. The band state deuterium forms a cooperative, collective matter phase called a Bose Bloch condensate (BBC), which infuses a host crystal, and in which the mean concentration of D^+ per unit cell is << 1. The properties of the BBC are those implicit in its many body wave function and the Fermi Golden Rule.

The BBC confers onto each unit cell of a crystal a low duty cycle transient occupation by single and multiple-occupation BBC deuterons. The wave function of these transient occupations reflects the zero point motion of interstitial deuterium. The multiple occupations are subject to reversible coalescence self-interactions in which there is a rapid fluctuation between chemical and nuclear density configurations. The nuclear density configuration of the 4-fold occupation state can decay into two 23.8 MeV alpha particles. Less certain, the double occupation state in Pd can result in successive scatterings of chemically bonded interstitial D, resulting in lattice heating without alpha particle decay.

Though the name Bose Bloch Condensate places special emphasis on the bosonic character of the D^+ ion, the Bose behavior of this particular "condensate" is only significant on the length and time scales associated with electrostatic interaction. The use of terminology that involves "Bose" and "condensate" in this context should not be confused with the more commonly used term "Bose Condensate". A Bose Bloch Condensate only resembles a "Bose Condensate" at low temperatures and only then on length scales that are much larger than nuclear dimension. At elevated temperatures, the bosonic nature of the BBC is important primarily because its presence means that the dynamics of each of the thermally accessible BBC states may be described in terms of a single, exchange-symmetrized many body wave function. The condensate aspect of the state refers to the fact that collectively the identity of each D^+ ion has been lost with respect to the others. The Bose Bloch Condensate is present at all temperatures in which each deuteron in a periodic host may be viewed as an independent particle that has become indistinguishable from a macroscopic number of other deuterons.

Our statement that the formation of band state D^+ becomes favorable in β PdD_x at x~1 is based on the following reasoning. The chemical potential for the reaction $D^+ + PdD_x \rightarrow PdD_{x+\varepsilon}$ has been described by Wicke and Brodowsky[7] as the sum of four terms, involving a single statistical term and three energy terms. These authors provide a figure which illustrates how the behavior of these four factors contribute to the chemical potential as x varies between 0 and 1. The statistical term shows the effect of the availability of unoccupied unit cells. It is negative at low x and positive as $x \rightarrow 1$. The energy terms include a zero point motion term, which is endothermic and independent of x, an electrostatic interaction term, which is exothermic at low x and becomes endothermic as $x \rightarrow 1$, and a lattice strain energy term, which is endothermic at low x and exothermic as $x \rightarrow 1$. The electrostatic term includes the summed effect on the system energy of: (1) adding a D^+ charge to the center of an octahedron whose vertices are Pd atoms, (2) adding an electron to the pool of Pd conduction electrons, and (3) rearrangement of electron charges associated with the conduction electrons so as to provide neutralization of the added D^+ ion. The term is exothermic at low x, where vacancies exist in the Pd 4-d electron band, and becomes increasingly endothermic when these vacancies become filled and the electrons are forced to occupy higher energy 5-s band states. The term we are most interested in, however, is the lattice strain term. This term is positive at low x since the addition of isolated D^+ ions to the lattice forces expansion of isolated unit cells in a lattice whose lowest energy condition occurs with unit cells of smaller size. The term becomes negative as $x \rightarrow 1$ because most unit cells are then occupied and only isolated cells are unoccupied. The lattice strain caused by the isolated unoccupied cells is relieved as D^+ is added, resulting in energy release.

One now asks the question: what happens when highly non-equilibrium electrochemistry forces D^+ ions into a stoichiometric PdD crystal. If additional D is to be added in the form of a normal chemical occupation of a unit cell, isolated unit cells must become doubly occupied, and the lattice strain energy term jumps from strongly exothermic to strongly endothermic. However, if the added D^+ ion can enter a band state and be shared by all the unit cells of the crystal, it will contribute only a fractional charge (ε <<1) to each unit cell of the lattice and all unit cells will be affected equally. As

a result the endothermic lattice strain energy cost is avoided. For this reason the band state D^+ is favored for the non-stoichiometric component of $PdD_{1+\varepsilon}$. Because this process involves an "overcharging" of the electrode by effectively adding a small amount of D^+, accompanying this condition will be a polarization of the charge in opposition to the normal charge flow prior to the overcharging. This polarization is the origin of the over-potential condition that is seen during the observation of anomalous heating.

Consider now the statement that band state D^+, which we call Bose Bloch Condensate D^+, or BBC D^+ is a cooperative, collective matter phase whose properties are determined by its many body wave function. It is standard solid state physics practice to describe band state electrons in terms of a set of collective states characterized by many body wave functions. The wave functions are fabricated from sums of products of single particle wave functions, with the sums made up of permutations of an initial set of wave function products, and with signs applied to the products to reflect the antisymmetry of the fermion wave function of the electron under particle exchange. The same procedure is applicable to band state deuterons, except that all component wave functions are positive, reflecting the symmetric wave function of D^+, which is a boson. This procedure reflects the existence of collective states formed from indistinguishable particles and is simply the application of the exchange principle to multiparticle states. For both band state electrons and band state deuterons the electrostatic potential controlling the collective state is periodic and imposes Bloch symmetry on the single particle wave functions, and thus also on the many body wave function describing the collective state. The Bose character of the D^+ band system impacts the behavior of the collective state mainly by its removal of the Pauli exclusion principle. As a result the collective states have high degeneracy and can support cooperative behavior. In the limit of low temperature, only a single state of the band system is occupied, and a fully cooperative condensate, exhibiting ionic superconductivity, is to be expected.

The statement that the BBC confers onto each unit cell of a crystal a low duty cycle transient occupation by single and multiple-occupation BBC deuterons is a reflection of the quantum field character of the many body cooperative state, and the fundamental wave-particle duality of quantum mechanics. The time-independent description of the BBC is in terms of Bloch functions (defined by Eq. 8), which are wavelike and have equal amplitude distributions over each of the unit cells of the crystal. The Bloch functions are the eigenstates of the BBC and their density integrals show an equal and fractional charge contribution to each unit cell. However, the many body wave function can just as well be expressed in terms of Wannier functions, which describe the BBC in terms of transient, low duty cycle, single particle occupations of each unit cell of the crystal. When the many body Bloch wave functions are expanded in terms of Wannier functions, the new expression has terms corresponding to both transient single particle occupations, and transient multiple particle occupations of each unit cell. The transient multiple particle occupation terms in the many body wave function are the source of the nuclear self-interactions predicted by our theory.

The mathematics associated with these transient multiple particle occupations can be understood by writing the many-body wave function first in terms of Bloch states $\psi_{\mathbf{k}}(\mathbf{r})$ and then rewriting each Bloch state in terms of Wannier states $\Phi_s(\mathbf{r_m})$. Specifically if we use the symbol (ε_p,r) to denote the set of all of the many-body spatial coordinates $\{r\}$ and occupied energy bands $\{\varepsilon_p\}$, the many-body wave function $\Psi(\varepsilon_p,r)$ is given by

$$\Psi(\varepsilon_p,r) = (1/N_B!)^{1/2} \sum_{\{\mathbf{r_m}\}} \{ \prod_{m=1}^{N_B} \psi_{\mathbf{km}}(\mathbf{r_m}) \} \qquad ,(9)$$

where N_B is the number of BBC bosons in the crystal, and the sum over $\{\mathbf{r_m}\}$ includes interchange of each coordinate $\mathbf{r_m}$ with the remaining N_B-1 coordinates, ensuring that Ψ is suitably Bose symmetric. Then, we may rewrite each Bloch state $\psi_{\mathbf{km}}(\mathbf{r_m})$ in terms of Wannier states $\Phi_s(\mathbf{r_m})$.

$$\psi_{\mathbf{km}}(\mathbf{r_m}) = (1/N_L)^{1/2} \sum_{s=1}^{N_L} \Phi_s(\mathbf{r_m}) \exp(i\mathbf{k_m}\cdot\mathbf{R_s}) \qquad ,(10)$$

where N_L is number of unit cells in crystal. Substituting Eq. 10 into Eq. 9, we find

$$\Psi(\varepsilon_p,r) = (1/N_B!)^{1/2} \times \sum_{\{r_m\}} (1/N_L)^{N_B/2} \{ \prod_{m=1}^{N_B} \sum_{s=1}^{N_L} \Phi_s(r_m) \exp(ik_p \cdot R_s) \} . \quad (11)$$

In Eqs. 10 and 11, $\Phi_s(r_m)$ is a Wannier function for boson **m** occupying unit cell **s**. In the harmonic approximation, it is appropriate to construct each Wannier function, at time t=0, using the ground state wave functions of a harmonic well whose curvature is defined by the classical turning point **a** of the motion.

$$\Phi_s(r) = (2/\pi a^2)^{3/4} \exp(-(r_s-r)^2/a^2) \quad (12)$$

Most of the terms in the bracketed product of sums of terms in Eq. (11) contain products in which the unit cell designator **s** is not repeated, since $N_L >> N_B$. A small fraction of the terms contain products in which the unit cell designator **s** is repeated twice. These terms describe double occupation of unit cell **s**. These terms contain factors $\Phi_s(r_m)\Phi_s(r_n)$, each of which is a product of cospatial wave functions centered on the center of unit cell s. Similarly, there are terms in which **s** is repeated three, four,....N_B times, corresponding to occupations of the unit cell **s** by three, four,...N_B deuterons. In each of these multi-particle occupations, each Wannier function has the same spatial distribution about the center of its unit cell, reflecting the zero point motion of a D^+ ion in the 3-dimensional potential well provided by the lattice. The collection of terms containing products corresponding to more than one deuteron occupying unit cell **s** are the only terms which contribute to nuclear self-interactions in unit cell **s**. They form the active portion of the input function to the Fermi Golden Rule expression as applied to unit cell **s**.

Both single and multiple occupation Wannier function products are transient due to the electrostatic self-interaction energy associated with unit cell occupation. The lifetime of each of the transient states is set by the Planck uncertainty principle $\Delta E \cdot \Delta t \sim h$. The uncertainty principle permits a short duration violation of the conservation of energy. The electrostatic self-interaction energies are calculable from the spatial distribution of the Wannier states, and are about 80 eV and 400 eV for the double and quadruple occupation states. The corresponding lifetimes are 5×10^{-17} and 1×10^{-17} s.

The statement that the wave functions reflect the zero point motion of D^+ ions in the lattice was discussed in conjunction with the ion cluster fusion observation.

The statement that multiple occupations of unit cells are subject to coalescence self-interactions between chemical and nuclear density configurations follows from: (1) the Fermi Golden Rule, (2) the cospatial form of the wave function products that are part of the initial state in the Fermi Golden Rule, (3) the existence of a nuclear interaction potential between paired neutron-proton elements in a nuclear density final state, and (4) our use of interaction potentials that are constructed from self-interaction in the limit in which electrostatic self-interaction and nuclear self-interaction occur on sufficiently different length and time scales that Born-Oppenheimer separability can be applied in the construction of the interaction potential and in the initial state. Because the quadruple and double occupancy electrostatic self-interaction energies (80 and 400 eV) are considerably smaller than the associated nuclear self-interaction energies (~10's of MeV), Born-Oppenheimer separability does apply to the initial state wave function, and in the construction of the interaction potential. (In the construction of the interaction potential associated with the quadruple particle case, it is necessary to perform an expansion about the center of mass of the four particle fluctuation in order to regroup terms in a suitable manner in which the rapidly and slowly varying contributions to the self-interaction become identifiable.)

The simplest mode of energy release through nuclear interaction that is consistent with momentum conservation and the selection rule in which the fusion products only involve configurations constructed from proton-neutron pairs when the initial state consists of deuterons is the coalescence reaction initiated from the quadruple occupation a site. In the limit in

which Born-Oppenheimer separability can be applied both to the reactants and the interaction potential, such a quadruple occupation provides an initial step in the decay of a virtual $^8Be^*$ nucleus to two alpha particles. We use the Fermi Golden Rule expression,

$$N = 2\pi/\hbar \; \Sigma \langle i|V|f\rangle \langle f|V|i\rangle \; \delta(E_i - E_f)$$

to calculate the associated reaction rate; N is the number of reactions per second within the crystal. This expression has been evaluated for a square well nuclear potential and a Gaussian input wave packet.

The possible modes of energy release through nuclear interaction that are consistent with momentum conservation and the selection rule in which the fusion products only involve configurations constructed from proton-neutron pairs when the initial state consists of deuterons are:

1) fusion via a nuclear configuration resembling $^8Be^*$, in which two 23.8 MeV alpha particles are released,

$$4D^+ \rightleftarrows {}^8Be^* \rightarrow 2 \text{ alpha} + 47.6 \text{ MeV}, \quad (13)$$

and

2) deexcitation of virtual $^4He^*$ states (associated with double deuteron [i.e., di-deuteron] occupation) through scattering between BBC di-deuterons with chemically bonded D. Schematically, the formation of such $^4He^*$ virtual states occurs through reversible coalescence reactions, of the form

$$2D+ \rightleftarrows {}^4He^* \quad (14a)$$

The subsequent deexcitation of these virtual states through scattering processes involving the chemically bonded D may occur through a series of scattering events:

$$^4He^* + D_{lattice} \rightarrow {}^4He^{**} + D_{lattice,scat} \quad (14b)$$

$$^4He^{**} + D_{lattice} \rightarrow {}^4He^{***} + D_{lattice,scat} \quad (14c)$$

. . . . . .

$$^4He^{**\cdots *} + D_{lattice} \rightarrow {}^4He + D_{lattice,scat} \quad (14d)$$

Here, each additional asterisk (in $^4He^{**\cdots *}$) is used to denote deexcitation of the nucleus. The chemically bonded (i.e., non-BBC) D are denoted by $D_{lattice,scat}$. (The chemically bonded deuterium refer to the D that are to be associated with the stoichiometric compound PdD.) Once reaction 14b takes place, the reverse reaction is blocked (even when the He state is virtual) through energy conservation. If one calculates the rate of Eq. 13 using the known size of the zero point motion of D^+ in PdD_x and assumes that the decay of the coalesced state into 2 alphas is prompt, then a BBC D^+ concentration of 3×10^{-7} BBC D^+ per unit cell is sufficient to produce the volumetric energy release of 10 W/cm^3 observed by Fleischmann and Pons[1].

However, it is not clear that alpha emission is the primary mode of energy release. It is probable that both the alpha particle emission mode (Eq. 13) , and the possible nuclear scattering mode involving virtual coalescence reactions from the double occupation state (Eq. 14a) could both be at work in the heating process . Scattering from the primary lattice constituent Pd also seems possible in imperfect crystals where wave function overlap occurs at lattice imperfections and at the crystal boundary. The nuclear scattering mode could liberate heat without release of any high energy particles. It is possible that the Li plays a role (as discussed in ref. 3) in a nuclear fashion, but it is probable that the most important impact of Li on the process is of an electronic nature, due to the Li-induced changes in surface chemistry. In regions where Bloch symmetry breaks down or is reduced, such as at interfaces, surfaces, or in other regions where periodicity is lost, it is to be expected that secondary reactions, initiated from the high energy D states (formed from Eqs. 14b-14d) will occur.

Finally let us consider experimental evidence for the validity of our theory. At last year's Utah meeting Chambers et al.[8] described a study in which a 130 A film of Pd sandwiched between two stainless steel diffusion barriers was loaded with deuterium by ion impact. The film was observed by a silicon particle detector. In two runs totaling a few hours a total of 8 abnormally high amplitude pulses were recorded. The 8 pulses could have been due to pick-up of unknown origin, as suggested by the authors, but if the pulses were due to high energy particles, the recorded energy losses averaged about 21

MeV. Our theory predicts emission of 23.8 MeV alpha particles. These authors also found a large number of low energy pulses due to response to a glowing ion-source filament. The lack of pulses outside the 21 MeV region supports the validity of the alpha particle interpretation.

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