## Excess Energy and Nuclear Products

# Radiationless Cold Fusion: Why Small "Crystals" Are Better, $N_{cell}$ Requirement, and Energy Transfer to Lattice

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Abstract
The Ion Band State Theory describes Fleischmann and Pons cold fusion phenomena. It is based on application of solid state band theory physics, many-body physics, and the known quantum behavior of hydrogen in metals. Important assumptions are that charge neutrality exists in each unit cell and that the reactive quantum states, which are stationary Bloch states, are describable as symmetric sums over complete sets of non-stationary, particle-like Wannier states. Consequences are that $D^+$-$D^+$ wave function overlap occurs for crystals possessing a sufficiently large number $N_{cell} > \sim 10^4$ of unit cells. Once this condition is met, small crystals provide more power per cc than larger crystals. Energy-transfer from the product state to the lattice electrons results from a change in the quantum of mass and resulting inelastic scattering due to charge distribution changes in the boundary region. The theory also predicts that the primary product is $^4$He, as observed.

Observations of Fusion in PdD$_x$ Explained by Ion Band State Theory
This paper is concerned with theory developed to explain Fleischmann and Pons (FP) type cold fusion. FP cold fusion is radiationless. Despite much study there has been no direct link established between emission of particles or $\gamma$-rays and the observed production of heat in PdD$_x$. This lack of radiation distinguishes FP cold fusion from muon catalyzed cold fusion and from any fusion that might occur due to transients producing "temperatures" and/or densities enabling hot fusion reactions.

FP cold fusion theory must take into account at least 3 other realities. Cold fusion does not occur in $D_2$ or any deuterided molecules. It is restricted to metals to which deuterium has been added, i.e., to deuterided metal lattices. Second, there is the substantial evidence provided by Arata and Zhang[1] that deuterided ultrafine Pd powder produces substantial heat under conditions that correspond to lower deuterium chemical potential than those employed by Fleischmann and Pons. Third, Arata and Zhang have established that $^4$He is the primary, if not sole, nuclear product.

The Ion Band State (IBS) Theory[2] has had singular success in providing a framework that can explain radiationless release of nuclear energy. This paper describes the IBS Theory and summarizes its assumptions. These assumptions include rules that are based on how quantum mechanics can apply in a periodic lattice in order for the effect to take place. They are not meant to be a minimum set of requirements for FP cold fusion; alternatively they could be incomplete. However, acceptance of the assumptions seems to lead logically to the conclusions (1) that there is a minimum "crystal" size enabling fusion, (2) that at significantly larger crystal sizes small crystals are better, (3) that there are

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symmetry-preserving means by which available nuclear energy can by dissipated in deuterided metal lattices without radiation, and (4) the nuclear product is $^4$He.

Language Problems: Different Names for Same Thing

Before discussing IBS theory, we address a language problem that may have confused readers of our earlier papers. We have used different names from different disciplines to describe the same thing. Equivalent names are listed below with the ones most used in this paper listed in bold type:

**deuteron = d = D⁺ = D⁺ ion** = deuterium nucleus

**stationary state = eigenstate** = time-independent state

**density distribution function** $= |\psi(r)|^2$ = probability distribution function for Compton scattering type interactions = "ion orbital"

**band state = Bloch function state** = **Bloch state** = [state for which $|\psi(r+R_n)| = |\psi(r)|$]
= [state for which $|\psi(r+R_{Bravais})| = |\psi(r)|$] = periodic amplitude state = lattice symmetric state = state having unbroken lattice symmetry = wavelike state = state resembling a standing wave = "periodic" state

Also, we use the term D⁺$_{Bloch}$ to mean a deuteron in a Bloch function state, i.e., with a spread-out charge distribution and having periodic symmetry.

Ion Band States on Surfaces

Both experiment and theory have shown that some of the excited states of hydrogen ions on metal surfaces are ion band states[3]. Also, ground state hydrogen on the relatively closely packed (111) surface of Ni appears to be a band state. The ground state hydrogen distributions on Ni (100), (110), and (111) have been calculated by Puska and Nieminen (1985). These calculations assume that the ion
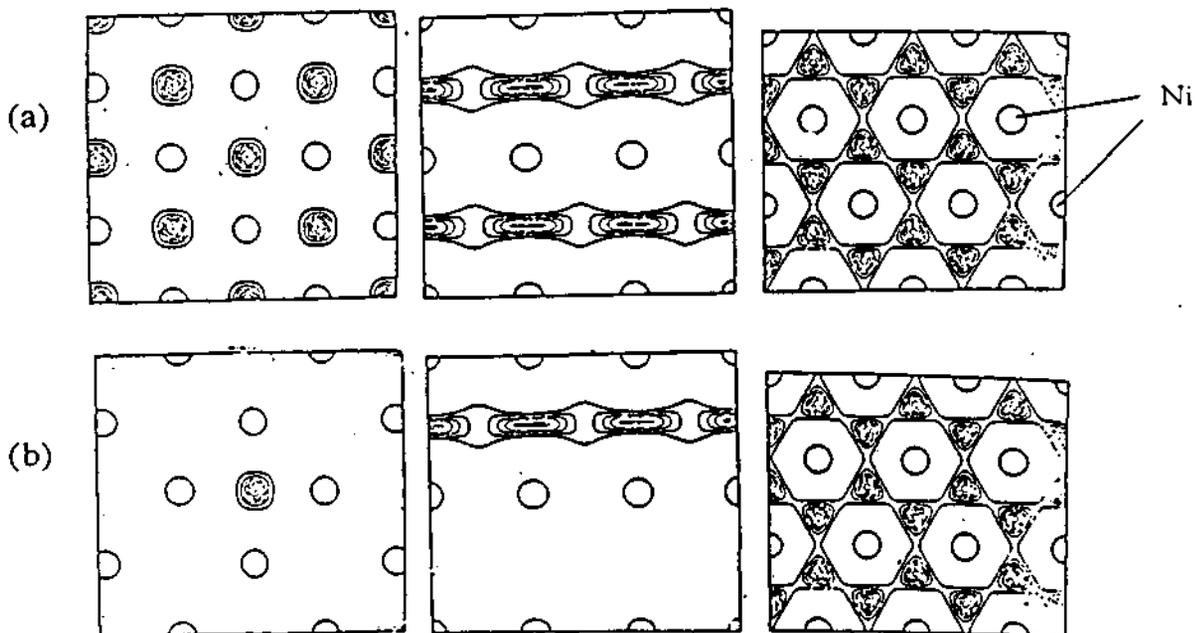


Fig. 1. (a) Calculated lattice-symmetric ground state H⁺ density distributions on Ni (100), (110), and (111) taken from Nieminen (1992)[3]. (b) Distributions reachable from a localized particle configuration.

wave functions are Bloch functions. In Fig. 1 we use these calculations to show the difference between localized (chemical) states and ion band states. We also show how, when H⁺ is locally

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deposited on a surface, the wave function can remain localized, or alternatively, if the localized configuration sufficiently overlaps its neighbor, the wave function can spread out over the metal's surface so that the $H^+$ becomes uncertain in its position. The $H^+$ then becomes, or transitions to, a band state ion, effectively having unbroken lattice symmetry.

The plots in Fig. 1 illustrate 1- and 2-dimensional band states. The FP reaction in $PdD_x$ is believed to be a 3-dimensional band state reaction, although the theory also applies to 2-dimensional states. The states supporting FP cold fusion will be assumed to be 3-dimensional.

Assumptions of the Ion Band State Theory
1. The active ingredient undergoing fusion is "paired" band-state deuterons which are part of a matter system described by a many-body wave function.
2. The system is describable by Schroedinger equation quantum mechanics as applied to indistinguishable particles. The 2-body point-particle correlation is fully described by the 2-body wave function.
3. "Paired" band state deuterons are describable by a 6-degrees-of-freedom 2-ion Bloch function in "center-of-mass, separation" coordinates. The Bloch condition applies to both "center-of-mass space" and "separation space".
4. The quantum mechanics superposition[4] principle applies in the sense that the 2-particle stationary state can be expressed as a sum over particle-like states, i.e. Wannier states[5] (virtual states in which identifiable whole ions occupy identifiable unit cells. Wannier states lack periodic symmetry.).
5. Each unit cell has net neutral charge.
6. The effect of electron screening on the stationary state is described by its effect on the 2-ion Wannier states, in accord with Assumptions 4 and 5.
7. Fusion rates can be calculated by time-dependent perturbation theory, which uses stationary initial and final state wave functions.
8. The nuclear and electrostatic portions of the stationary 2-ion wave function preserve a symmetry requirement that it be impossible to identify a specific location of a nuclear reaction.
9. The nuclear reaction couples to the lattice through a coherent release of energy and redistribution of small but equal amounts of charge from each unit cell within the bulk to the surface boundary region.

How Process Works
Broadly speaking, FP cold fusion occurs because deuterons occupying band states have their charge spread out and subdivided within a dominating periodic potential provided by a metal crystal. The IBS process does not work by confining 2 deuterons to a small volume, such as occurs in muon-catalyzed fusion. The IBS process requires that only a small fraction of the deuterons in $PdD_x$ ($< 0.0001$) be in Bloch configuration states to explain observed power rates.

Properties of Quantized Matter
Sometimes quantum mechanics is described as attributing a mix of particle-like and wave-like properties to matter. Such a picture is appropriate for unbound particles. Here we describe quantum mechanics applied to bound systems as attributing a mix of particle-like and quantized-matter-field-like properties to matter. Sometimes quantized matter is mostly particle-like with some matter field properties. Sometimes quantized matter is mostly field-like with some particle-like properties. These behaviors are illustrated in Fig. 2, using modifications of the surface band state distributions calculated by Puska and Nieminen.

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It is important to note that both distributions 2a and 2b apply to a <u>single</u> band state H$^+$ ion. The second key point to note is that 2b and 2d show single particles and double Bloch-function particles as having identical distributions in space on Ni (111). This behavior would be expected if there were no D$^+$$_{Bloch}$-D$^+$$_{Bloch}$ repulsion. However, it is also true, as we will show, if the D$^+$$_{Bloch}$-D$^+$$_{Bloch}$ repulsion is sufficiently weak, provided that the assumptions of the IBS Theory apply.

<u>H on Ni (100) is particle-like</u>         <u>H on Ni (111) is field-like</u>

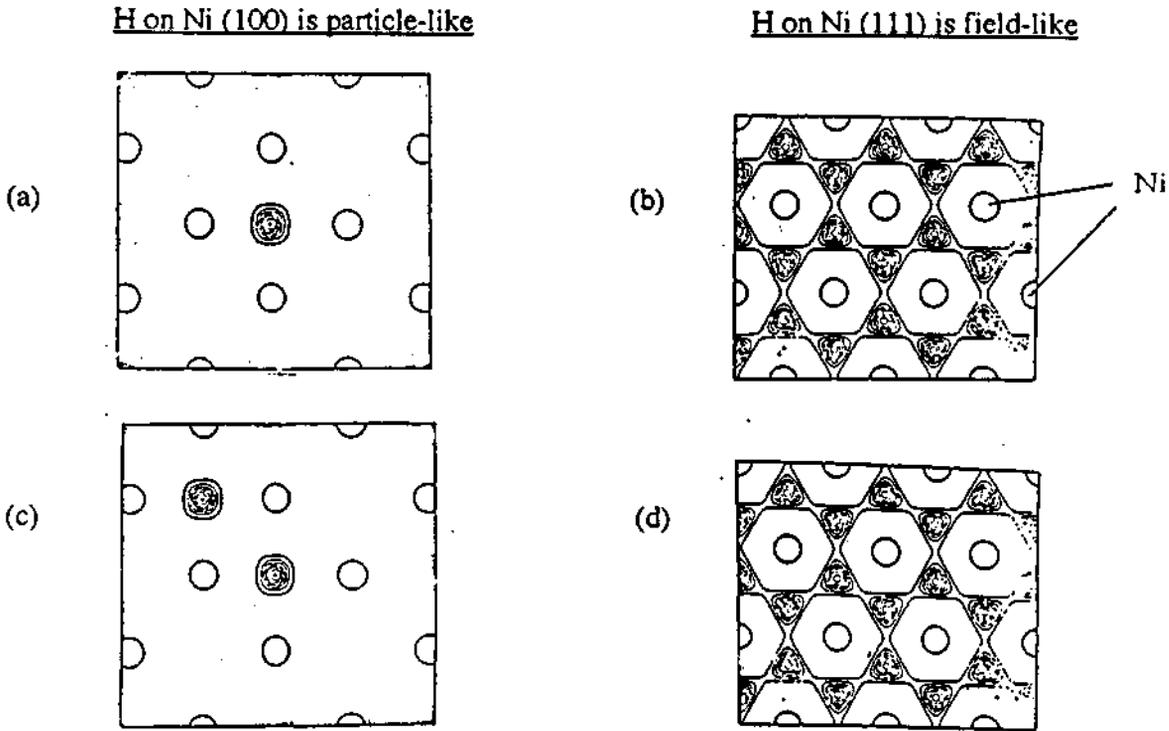(a)         (b)       Ni

(c)         (d)

Fig. 2 Calculated charge density distributions of H$^+$ on Ni surfaces. (a) Single proton on Ni (100); (b) Single proton on Ni (111); (c) Two adjacent protons on Ni (100); (d) Di-proton on Ni (111)

<u>The 2-D$^+$ Band State Wave Function</u>
If the D$^+$ see only the periodic potential of the lattice and one neglects D$^+$-D$^+$ repulsion, the exchange-symmetrized Schroedinger 2-body band state wave function is:

$$\Psi\,(r_1,r_2) = \frac{1}{\sqrt{2}}\left[\psi_1(r_1)\ \psi_2(r_2)\ +\psi_1(r_2)\ \psi_2(r_1)\right]\quad.$$

Here we are assuming that the periodic symmetry imposed by the lattice requires that $\Psi$ ($r_1,r_2$), $\psi_1(r_1)$, and $\psi_2(r_2)$ be Bloch functions. $\Psi$ ($r_1,r_2$) is a function of 6 dimensions (6 degrees of freedom), i.e., $r_1$ and $r_2$ are independent vector variables. IBS theory assumes that $\psi_1$ and $\psi_2$ are independent functions. The Bloch function requirement then means that the amplitude distribution $|\Psi(r_1,r_2)|$ does not change if $r_1 \rightarrow r_1 + R_i$ and/or $r_2 \rightarrow r_2 + R_j$. Here $R_i$ and $R_j$ are independent Bravais lattice vectors.

When D$^+$-D$^+$ repulsion is included but kept weak, and provided each D$^+$ is screened by its neutralizing charge on length scales that are small compared to unit cell dimensions (which is true for two IBS D$^+$ in PdD), $\Psi$ can be expressed in terms of position, separation vectors $r_{cm} = (r_1+r_2)/2$ and $r_{12} = r_1 - r_2$.

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$$\varphi(\mathbf{r}_{cm}, \mathbf{r}_{12}) = \psi_{cm}(\mathbf{r}_{cm})\; g_{12}(\mathbf{r}_{12}) \qquad ,$$

where $\psi_{cm}$ and $g_{12}$ are Bloch functions, i.e., $|\psi_{cm}(\mathbf{r}_{cm}+\mathbf{R}_n)| = |\psi_{cm}(\mathbf{r}_{cm})|$; $|g_{12}(\mathbf{r}_{12}+\mathbf{R}_m)| = |g_{12}(\mathbf{r}_{12})|$; and $\mathbf{R}_n$ and $\mathbf{R}_m$ are independent lattice vectors. Here vector $\mathbf{r}_{cm}$ defines a position in real space. Vector $\mathbf{r}_{12}$ defines a separation magnitude and direction in "separation space". As required by Schroedinger quantum mechanics for the general 2-particle case $\varphi(\mathbf{r}_{cm}, \mathbf{r}_{12})$ has 6 degrees of freedom. The assumptions that $\varphi(\mathbf{r}_{cm}, \mathbf{r}_{12})$, $\psi_{cm}(\mathbf{r}_{cm})$, and $g_{12}(\mathbf{r}_{12})$ are Bloch functions is in accord with Assumption (3) of the IBS Theory. This condition is consistent with the assumed independence of Bloch functions $\psi_1(\mathbf{r}_1)$ and $\psi_2(\mathbf{r}_2)$ in the normal configuration-coordinate formalism of the Schroedinger theory. $\varphi(\mathbf{r}_{cm}, \mathbf{r}_{12})$ is a function of 3 dimensions of real space and 3 dimensions of separation space.

The Bloch function requirement for $g_{12}(\mathbf{r}_{12})$ means that the interaction point $\mathbf{r}_{12} = 0$ is repeated in each unit cell of separation space, since $g_{12}(\mathbf{R}_m) = g_{12}(0)$ where $\mathbf{R}_m$ is any Bravais lattice vector in separation space. The points $[\mathbf{r}_{12} = 0, ..., \mathbf{R}_m, ...]$ are thus assumed to be coherently linked (as a consequence of periodic, order-preserving symmetry) in separation space, as are points $[\mathbf{r}_{cm}, ..., \mathbf{r}_{cm} + \mathbf{R}_n, ...]$ in real space.

In the $\psi_{cm}(\mathbf{r}_{cm})\, g_{12}(\mathbf{r}_{12})$ representation, $|\psi_{cm}(\mathbf{r}_{cm})|$ is called the "matter-field strength" and $|\psi_{cm}(\mathbf{r}_{cm})|^2$ is called the "matter-field density". The quantity $e\,|\psi_{cm}(\mathbf{r}_{cm})|^2$ is the charge density. $g_{12}(\mathbf{r}_{12})$ is called the "dimming function". $|g_{12}(\mathbf{r}_{12})|$ modulates the amplitude of wave function $\varphi$ everywhere in real space based on the value of $\mathbf{r}_{12}$ in separation space. $g_{12}(\mathbf{r}_{12})$ is also called the "cusp function" because it has a cusp at $\mathbf{r}_{12}=0$ and all equivalent points.

## Visualization of the 2-D⁺ Band State Wave Function

It is helpful to have a visual representation of the 2-D⁺ band state wave function $\varphi(\mathbf{r}_{cm}, \mathbf{r}_{12}) = \psi_{cm}(\mathbf{r}_{cm})\, g_{12}(\mathbf{r}_{12})$. Since $\varphi$ has 6 degrees of freedom, it is best shown in two 3-dimensional drawings. To simplify the author's task, each of these 3-dimensional drawings is illustrated by a sketch of wave function amplitude versus position along a line through an idealized crystal lattice. This amplitude vs. position function is shown in Fig. 3a. This selected line is taken to pass through a sequence of saddle points in the electrostatic potential provided by the lattice. The saddle points are the minima in the potential barrier that localized interstitial D⁺ ions must overcome to diffuse through the crystal. The accompanying dimming function in separation space is shown in Fig. 3b.
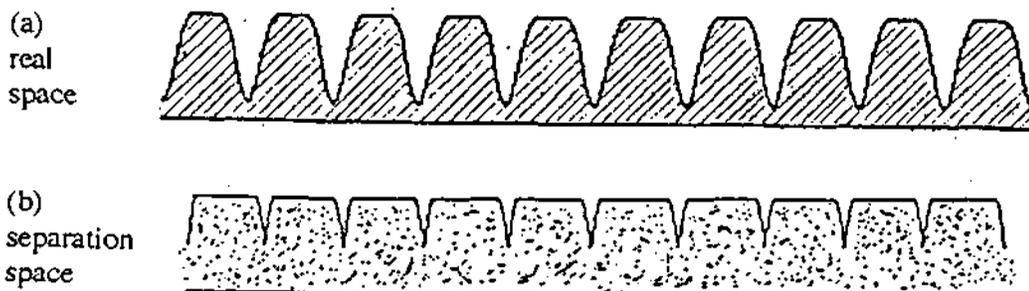
(a)
real
space



(b)
separation
space



Fig. 3. (a) $|\psi_{cm}(\mathbf{r}_{cm})|^2$ vs. position $\mathbf{r}_{cm}$ along a line through a row of saddle points in an idealized cubic lattice. $\mathbf{r}_{cm}$ describes positions in real space inside a metal crystal lattice. (b) $g_{12}(\mathbf{r}_{12})$ vs. separation vector $\mathbf{r}_{12}$. $|g_{12}(\mathbf{r}_{12})|$ reduces the amplitude of the 2-ion wave function $\varphi$ as $\mathbf{r}_{12} \rightarrow 0$. $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ is the separation between coherently linked particle positions.

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In the IBS Theory each reaction occurs throughout the crystal in real space and at $N_{cell}$ coherently-linked cusp points in separation space. The crystal is assumed to be made up of $N_{cell}$ identical unit cells.

The starting point for the IBS 2-ion wave function is the pure matter field picture that models the band state ions in a lattice when $D^+$-$D^+$ repulsion is neglected. Here a field means an entity that has a defined value at every point in 3-dimensional space, i.e., is a function of the position vector in real space. Only 3-dimensions are required to describe the matter field. As the $D^+$-$D^+$ point-particle repulsion is turned-on, the quantized matter field changes into a 6-dimensional 2-body wave function. A dependency in separation space is created and the cusps shown in Figure 3b begin to grow. If the repulsion potential is permitted to grow to its real value, cusps grow to a magnitude that is determined by minimization of total system energy. Calculations[2] show that the energy-minimizing cusp amplitude is a function of $N_{cell}$. The cause of the $N_{cell}$ dependence is a reduction in the point-particle interaction potential for Bloch function $D^+$ from its free space value, caused by the existence of multiple cusps in separation space. As described in ICCF5 (Chubb and Chubb, 1995) the point particle interaction potential calculated in accord with Assumptions 4 and 5 of the IBS Theory, which is appropriate for metals, is $e^2/(r_{12}N_{cell})$. Ideally, at some $N_{cell}$ lower limit less than $\sim 10^4$, the cusps reduce the amplitude of the wave function to zero and no wave function overlap and cold fusion can occur. With still smaller crystals the cusp picture is no longer valid and the energy-minimized wave function splits into a diatomic molecule-like configuration in which negligible overlap occurs. The $N_{cell}$ lower limit is the minimum $N_{cell}$ requirement for cold fusion.

## Why Small Crystals Are Better

Once metal crystals are sufficiently large that $N_{cell}$ exceeds the minimum value required for $D^+$-$D^+$ wave function overlap and fusion, still larger crystals are detrimental in that they reduce heat production per cc. This reduction is a consequence of the matter field character of the FP fusion reaction. Effectively, because the reactant is derived from the 2-particle terms in the many-body wave equation describing a $D^+$ matter field which is confined to a single crystal, each crystal is a separate reactor. The other important factor is microscopic reversibility, which is expressed in the interaction matrix element identity $|V_{if}| = |V_{fi}|$ of the Fermi Golden Rule reaction rate equation. Microscopic reversibility means that the final state is as important as the initial state in reaction rate calculations. The final state wave function corresponds to a field strength of one $^4He^{++*}{}_{Bloch}$ excited-product Bloch function ion per crystal, regardless of crystal size. At the same $D^+{}_{Bloch}$ concentration per unit volume, each crystal produces heat at the same rate per crystal. Since each crystal produces the same heat, the more crystals per cc, the higher the heat generation rate per cc. However, as described previously[2], the theory may not be applicable for crystals with $N_{cell} < 10^9$, because only when $N_{cell} \gtrsim 10^9$ is sufficient periodic order present to justify in a rigorous fashion that the ion band state theory apply.

## d-d "Field" Reaction Rates; (Self-Interaction Reactions of a Matter Field)

Here we show more details for 2-particle matter field self-interaction fusion reactions. Reaction rate is calculated on a per-crystal basis. The matter field density is expressed in terms of normalized wave function densities. The matter field density of each particle integrated over a unit cell is $1/N_{cell}$ because each particle wave function is normalized at 1 particle per crystal. Hence the field of each particle decreases with crystal size, but the number of pairs equally increases with crystal size. The result of the calculation is described below:

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Reaction Parameters::

$\dot{N} \equiv$ [reactions s$^{-1}$ crystal$^{-1}$]

Field pair-density of 2-D+$_{Bloch}$: $|\psi_{cm,ij}|^2$. Fraction of deuteron pair$_{ij}$ per unit cell $\propto |\psi_{D,i}|^2 \, |\psi_{D,j}|^2$
$$= 1/N_{cell}^2$$

Field density of $^4$He$^{++}$*$_{Bloch}$: 0 in initial state

$|\psi_{cm,He}|^2$ in final state. Fraction of He per unit cell $= 1/N_{cell}$

Reactions rate per unit cell

$$
\frac{\dot{N}}{N_{cell}} \quad
\begin{array}{cccc}
\propto & |\psi_D|^4 & |\psi_{He^*,\,final}|^2 & \text{number of pairs} \\[4pt]
\propto & 1/N_{cell}^2 & 1/N_{cell} & N_D(N_D-1) \\[4pt]
\tilde{\propto} & 1/N_{cell}\; c_{D,Bloch}^2 & s^{-1}\;\text{unit-cell}^{-1} &
\end{array}
$$

Reaction rate per crystal

$$\dot{N} \;\tilde{\propto}\; c_{D,Bloch}^2 \quad [s^{-1}\text{ crystal}^{-1}]$$

We have used the approximation $N_D^2 \cong N_D(N_D-1)$ and the relation $N_D = c_{D,Bloch}\,N_{cell}$. Concentration $c_{D,Bloch}$ is the number of D+$_{Bloch}$ per unit cell. Both initial and final state field densities enter the reaction rate per unit cell because of quantum mechanics microscopic reversibility, which appears in the Fermi Golden Rule reaction rate equation. To get the reaction rate for the crystal as a whole we have summed over the unit cells in a single crystal.

Because the fusion rate is the same for big and small crystals, the smaller the crystals, the more fusions per cc.

Heat Generation: Coupling between the Nuclear Reaction and the Lattice
In a quantized matter field as shown in Figs. 2 and 3, paired D+ as seen in each unit cell are constrained relative to each other to a volume of atom/molecular dimension, as opposed to nuclear dimension. Because energy minimization has eliminated the coulomb barrier, the remaining strong force attraction between antiparallel nuclear spin deuterons leads to coalescence[2] (i.e., to a reversible form of the interaction matrix element $|V_{if}|$) by which the nuclear components of the wave function are constrained relative to each other to a volume of nuclear dimension. This coalescence is reversible until some small amount of energy is transferred to the lattice. The $^4$He$^{++}$*$_{Bloch}$, which is the product of the coalescence (Chubb and Chubb, 1991), constitutes a new matter field which has a different quantum of mass and a different set of Bloch eigenstates than those of the D+$_{Bloch}$. The coalescence process occurs coherently throughout the crystal, and occurs equally and simultaneously in each unit cell and in the boundary region. As an example of volume change, if the change from mass-2, charge-1 to mass-4, charge-2 occurred for ions in a 3-dimensional harmonic well, the decrease in volume of the ground state wave function would be a factor of 8.

It is assumed that the coalescence process occurs without disturbing periodic order and without altering the charge distribution within the crystal bulk. However, in the boundary region, which is coherently connected to the bulk, there is a change in charge distribution caused by the reduced coherence length associated with the $^4$He$^{++}$*$_{Bloch}$ quantum of mass. To be specific, the ion wave

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function in the boundary region, which is required to match the bulk solution at the surface, is forced to die out by a rising potential on opposite sides of the bulk. In this rising barrier region the $^4He^{++*}$ wave function falls off more rapidly than the $D^+$ wave function at locations extending away from regions corresponding to the lower potential that characterizes the crystal bulk.

Throughout the crystal the band state ions are coupled to the many-body electron system which provides the potential minimum within which the $D^+$ reside in each unit cell. A change in the charge distribution within the boundary region inelastically scatters the band state electrons into empty states above the fermi level. The scattering process is the same scattering process that accompanies current flow (resistive heating). Once any electron scattering takes place, the reaction goes to completion in the boundary region with the release of energy in the solid totaling 23.8 MeV. The electron coherence volume extends beyond the ion coherence volume. As a result, for embedded crystals the many-body electron system extends beyond the ordered region of a single embedded crystallite and the heating effect extends beyond the $N_{cell}$ volume.

In addition to energization of the band state electrons, there is a transfer of the $He^{++}$ charge with its neutralizing electrons from the bulk to the boundary region, a slight shrinkage of the crystal, and a generation of phonons.

### Indirectly accessible Bloch states
A candidate state for FP cold fusion is a 3-dimensional analog of the $H^+$-on-Ni (100) Bloch state illustrated in the left panel of Fig. 1a. Such a state is not directly accessible, or not easily accessible, from a localized occupied state, but is indirectly accessible through the occupation of an overlapping spread-out state. Occupation from a more accessible spread-out, excited state (Arata's "spillover" deuterium?) should involve a heat of transition and impose strict Bloch symmetry on allowed selection rules. The transition would likely be exothermic. Calculated fusion rates would be higher than in more spread-out states because of a smaller occupied volume prior to coalescence. Difficulty of depopulating indirectly accessible Bloch states may be responsible for the FP "heat after death" phenomenon.[6]

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