COLD FUSION AS AN INTERACTION BETWEEN ION BAND STATES

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A theory of solid-state fusion based on the interaction between D^+ and $^4He^{++}$ ion band states within a host lattice is presented. Formation of ion band-state deuterium is thermo-dynamically favored when lattice strain energy is greater than the incremental chemical potential of the band state. The key fusion step is a coalescence fluctuation that converts a twofold occupation state of electrostatic zero-point-motion size into a state of nuclear dimensions. Rates are calculated using the Fermi Golden Rule. Fusion energy is shared between band-state members and subsequently transferred to the lattice.

INTRODUCTION

This technical note examines the possibility of nuclear potential-driven interactions between low-density ion band states formed within a host lattice. The candidate interaction is between D^+ and $^4He^{++}$ band-state populations. During the interaction, the D^+ band-state population is decreased by 2 D^+, and the $^4He^{++}$ band-state population is increased by unity. The nuclear reaction energy is shared at all lattice sites, in a distributed manner, by all members of both D^+ and $^4He^{++}$ band-state populations. The wave function overlap required for reaction is provided by the algebraic properties of the many-body band-state wave function, and *not* by tunneling, which is the basis of conventional nuclear physics. The reason that tunneling is not required is that, under suitable conditions (consistent with cold fusion electrolytic cell environments), occupation of the many-body band state becomes preferable energetically. Once the band state becomes occupied, overlap necessarily takes place.

BACKGROUND

The cold fusion phenomenon was discovered by Fleischmann and Pons[1] as a nonchemical production of heat during electrolysis of LiOD dissolved in D_2O using a palladium negative electrode. Liaw et al.[2] observed a larger nonchemical production of heat during electrolysis of LiD dissolved in a KCl-LiCl eutectic melt using a palladium positive electrode. The Liaw et al. cold fusion measurement was impressive in that heat production in deuterated palladium was successfully repeated, it showed a nonchemical heat output of ~12.5 times electrolytic power input, it showed sustained power output over a full day at 600 W/cm^3 Pd, with two additional days at somewhat lower power density, and the study included control observations in which little or no anomalous heat was observed when titanium was substituted for palladium or when LiH was substituted for LiD. The study established that cold fusion is not limited to low

temperatures and that lithium-in-palladium is not an initial part of the cold fusion process. Subsequent mass spectrometer analyses of the palladium electrode showed the presence of ^{4}He in concentrations not observed in an unused piece of palladium from the same source,[3] which indicates that ^{4}He is the probable nuclear reaction product.

The hypothesis that band-state D$^+$ is the reactant responsible for cold fusion was first proposed by Chubb and Chubb.[4-8] The initial reaction considered was the double-alpha-particle decay resulting from fourfold occupation terms associated with the many-body wave function of the D$^+$ band state. Although there is some evidence of ~21-MeV alpha-particle emission from deuterated palladium,[9] the source of primary heating is now believed to be a result of interactions between two band-state populations. High-energy particle emission is not believed to be part of the main energy release process. In support of the double-band-state hypothesis, there is evidence that processing palladium in helium improves its performance in the Fleischmann-Pons type of experiment.[10]

ION BAND STATES: THE BOSE BLOCH CONDENSATE

An ion band state, also called a Bose Bloch condensate (BBC), is a state of matter resembling a band-state population of electrons in a host solid, e.g., electrons in n-type silicon. Band states are collective populations of particles distributed throughout a crystal and described by a single many-body wave function. The ion band states responsible for cold fusion are formed from D$^+$ and ^{4}He^{++}, which have Bose rather than Fermi symmetry. These two ionic band states differ from electron band states in that their many-body wave functions require symmetric exchange symmetry (because the ions are bosons) and contain no explicit two-particle ion-ion correlation terms, such as are required, for example, in the description of the conduction electron population of sodium metal.[11] Ion-ion repulsion is included in the description of the BBC matter state as a perturbation of the many-body wave function, which interacts dominantly with the electrostatic potential provided by the host lattice.

The ion band states differ from most band-state electron populations in that very low ion concentrations are involved, probably $<10^{-6}$ band-state ions per unit cell.

THERMODYNAMIC ARGUMENT FOR ION BAND STATES WITHOUT EXPLICIT ION-ION CORRELATION TERMS

An ion band-state population exists in a host lattice if and only if the presence of such a population minimizes the free energy of the total system. The alternative to the formation of an ion band state is a normal chemical compound. In normal chemistry, ion-ion correlation terms keep nuclei apart and prevent nuclear interaction. The structural factor that favors formation of D$^+$ band states at low ion band-state population density is lattice strain energy.[12]

Lattice strain energy is the result of the differential expansion of the lattice that occurs when a unit cell becomes interstitially occupied. In beta-phase PdD$_x$ at low x, for example, the lattice strain energy μ_{strain} is endothermic and is ~0.19 eV per incremental deuteron.[12] Formation of band-state D$^+$ without explicit ion-ion correlation terms avoids this energy cost. The occupation of a band state causes no lattice strain energy because the band state populates all unit cells equally and hence does not require localized expansion of the lattice. There is, however, an ion-ion perturbation energy cost associated with the formation of band-state D$^+$. This cost occurs because formation of a band-state population of bosons requires, as a corollary, the presence of

terms in the many-body wave function that correspond to transient multiple occupations of unit cells of the host crystal lattice. These multiple occupations impose a self-interaction Coulombic repulsion energy cost. At low concentration in pure metal hosts, the double-occupation terms dominate this energy cost.

The fraction of time that any deuteron spends as a partner of a double occupation depends on concentration. At very low concentration, the fraction of time each ion spends in a double occupation is equal to the concentration c, where c is the number of band-state ions per unit cell. If E_2 is the endothermic (Coulombically induced) self-interaction energy for a doubly occupied cell, the energy cost per ion μ_{coul} for formation of the band state is cE_2. Thus, if c is sufficiently low, the band state is favored over the chemical state. We show that for D^+ ions, $E_2 \sim 80$ eV, so that for $c < 0.002$, the band state is favored.

The presence of explicit ion-ion correlation terms in the wave function is representative of the chemical state wave function. When explicit ion-ion correlation is included in the ion band state, for example, with inclusion of Jastrow factors[13] applied to the single-body wave functions used in forming the many-body wave function, the resulting structure resembles that of a Wigner solid. This imposes an approximately regular ion-ion spacing dependent on the concentration c and independent of the lattice spacing of the host. If one considers a PdD host and adds the requirement of space-charge neutralization, one is led to spaced interstitial D_2 molecules within a PdD host, similar to the configuration studied by Leggett and Baym.[14] This configuration resembles the low-concentration classical chemistry picture. If the host is a pure metal, such as silver, for example, the picture is that of separated interstitial deuterium atoms, analogous to that of beta-phase PdD_x. Both AgD_δ and $PdD_{1+\delta}$ ($\delta \ll 1$) have chemical configurations that impose a lattice strain energy cost μ_{strain} on the total system. The thermodynamic argument states that when $\mu_{coul} < \mu_{strain}$, band-state D^+ is the preferred configuration. Thus, since μ_{coul} is proportional to c, the band state should form at very low c, at least in pure metals. The cold fusion experiments indicate that it also forms when the host lattice is PdD. (To our knowledge, no serious attempt has been made to observe cold fusion in AgD_δ.)

WAVE AND PARTICLE CHARACTERIZATION OF A BBC

The components of a BBC are bosons in distributed matter states, i.e., Bloch states, which match the periodic symmetry of the host lattice. The bosons are indistinguishable. The many-body wave function describing the BBC is composed of many terms. Each term is composed of the products of all the individual particle Bloch wave functions. If a BBC in a crystal contains N_B bosons, each term of the many-body wave function is the product of N_B single-particle wave functions. The resulting characterization of the state is wavelike, and the characterization is the time-independent eigenfunction description of the BBC.

The nuclear instability of a D^+ BBC is more understandable in the particle-like representation of the same state. The particle-like representation is composed of products of Wannier functions,[15] which describe the BBC as a succession of transient integer occupations of unit cells. Contained in the algebra of the Wannier description of the BBC is the existence of transient multiple occupations of discrete unit cells. During the transient occupations, D^+-D^+ overlap occurs, with the result that there can then be a 2 D^+ overlap with a mass 4 nuclear density configuration. This overlap makes possible reversible, energy-conserving coalescence fluctuations between chemical and nuclear density configurations. If the D^+ spins are opposed,

the nuclear density configuration can be a $^4\text{He}^{++}$ nucleus. If the resulting $^4\text{He}^{++}$ is a part of a $^4\text{He}^{++}$ band state, the nuclear reaction energy is shared with all members of both the D^+ and $^4\text{He}^{++}$ band states. In a periodic solid, this form of reaction maximizes entropy in a manner consistent with maintaining periodic order. Subsequent disruptions of order increase the entropy of the system.

The particle-like representation of the BBC is no more real, nor less real, than the wavelike Bloch representation. The same overlap exists in the Bloch representation, but the picture is then of a steady-state fractional occupation of each unit cell. Integration must then be carried out over the entire number of unit cells N_L of the host crystal. The resulting overlap integral has the same value. The two representations are equivalent. For calculation of the chemical potential of the band state and for analysis of nuclear interaction rates involving final-state defect wave functions, we have used the particle-like representation.[4-8] For the analysis of the nuclear interaction rates involving final-state Bloch wave functions, we use the wavelike representation.

COLD FUSION IN A SILVER HOST

Silver is not known to form a stable hydride. Nonetheless, silver must be considered as a potential cold fusion host. It has the same face-centered-cubic lattice as palladium, and the same terms in the incremental chemical potential for hydrogen addition should apply. Wicke and Brodowsky[12] refer to the key exothermic term in the incremental chemical potential for PdH_x at low x as the electronic term. The electronic term is exothermic as long as the 4-d electron band state of palladium remains unfilled, but it becomes endothermic when most of the electrons added by deuterium injection are forced to enter 5-s bands. In silver, the 4-d bands are fully filled, and the electronic term is endothermic, explaining the lack of a stable hydride. If deuterium is injected into silver, or forced in by creation of a nonequilibrium surface deuterium atom concentration formed by nonequilibrium electrochemistry, the deuterium can either enter an unstable chemical interstitial state or form a D^+ band state. By our previous argument, a band-state population is probably favored at $c < 0.002$.

For definiteness, we envisage fusion in a silver crystal of 0.1-mm dimension. This crystal contains $N_L = 5.8 \times 10^{16}$ unit cells. We envision the crystal infused with 10^9 D^+ ions. Thus, $c = 1.73 \times 10^{-8}$. The wavelike description of the resulting BBC is that of standing waves with local maxima in each of the unit cells of the crystal. The energy $\varepsilon(\boldsymbol{k})$ of each band-state particle is a function of particle wave vector momentum $\boldsymbol{k}$, which is defined by Bloch's theorem:

$$\psi_{Bloch}(\boldsymbol{k}, \boldsymbol{r} + \boldsymbol{R}) = \psi_{Bloch}(\boldsymbol{k}, \boldsymbol{r}) \exp(i\boldsymbol{k} \cdot \boldsymbol{R}) \ , \tag{1}$$

where $\boldsymbol{R}$ is a Bravais lattice vector. In our model, we assume that there is both a D^+ band-state population consisting of N_D deuterons, and a $^4\text{He}^{++}$ band-state population consisting of N_{He} doubly charged helium ions. The cold fusion reaction consists of $N_D \rightarrow N_D - 2$ and $N_{\text{He}} \rightarrow N_{\text{He}} + 1$. The resulting 23.8-MeV energy release is shared by all of the $N_D + N_{\text{He}}$ ions, expressed as an increase in the available band energies. For $N_D \gg N_{\text{He}}$, the energy increase of each deuteron $\Delta\varepsilon_D(\boldsymbol{k})$ is ~0.02 eV. The deBroglie wavelength of a 0.02-eV deuteron is 1.43 Å. Heating of the lattice occurs when this energy is transferred from either BBC to the lattice by direct phonon coupling (or other direct coupling in which wave vector momentum is conserved), by indirect Umklapp processes (in which the solid as a whole recoils and wave vector momentum is changed by a reciprocal lattice vector), or by localized interactions at locations where periodic crystal symmetry is broken.

BBC FORMATION USING BOSONS THAT INTERACT ONLY WITH THE LATTICE

Consider first a BBC formed from mutually noninteracting bosons. These bosons interact only with a host metal lattice and its itinerant electron population. (Boson/boson interactions are treated later, as a perturbation.)

Let N_B bosons be distributed within a crystal containing N_L host unit cells. It is assumed that the bosons reside in potential wells within the unit cell of the host metal. Fractional charge is allowed at each site so that the potential provided by the lattice is periodic over a large enough scale that Bloch functions apply. The single-particle wave functions $\psi_{Bloch}(k,r)$, shown in Eq. (1), can be expanded in terms of Wannier functions[5]:

$$\psi_{Bloch}(k,r)\exp[-\epsilon(k)t/h]$$
$$= 1/N_L^{1/2} \sum_{s=1}^{N_L} \Phi_s(r,t)\exp(ik\cdot R_s) \ ,$$

(2)

where

R, R_s = Bravais lattice vectors

$\varepsilon(k)$ = band energy of ψ_{Bloch}

k = crystal momentum

Each Φ_s is a Wannier state, which, in the harmonic approximation, is suitably approximated at time $t = 0$ by the ground-state wave function of a parabolic well with zero-point energy E_0:

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

(3)

where

$$r_s = r - R_s$$
$$a^2 = 3\hbar^2/(m_B E_0)$$
$$\hbar = h/2\pi$$
$$h = \text{Planck's constant}$$
$$m_B = \text{deuteron mass for a D}^+ \text{ BBC.}$$

The many-body wave function (wavelike representation) associated with the occupation of N_B band states [denoted by the set of eigenvalues $\varepsilon_p = \{\varepsilon_p(k_m), m = 1, N_B \}$], possessing N_B coordinate dependencies r, is given by

$$\Psi(\epsilon_p, r) = (1/N_B!)^{1/2} \sum_{\{r_m\}} \prod_{m=1}^{N_B} \psi_{Bloch}(k_m, r_m) \ ,$$

(4)

where the sum over $\{r_m\}$ includes exchange of each coordinate r_m with the remaining N_B - 1 coordinates, ensuring that Φ is suitably Bose symmetric. Substituting Eq. (2) into Eq. (4), we find that

$$\Psi(\epsilon_p, r) = (1/N_B!)^{1/2} \sum_{\{r_m\}} (1/N_L)^{N_B/2}$$

$$\times \left[\prod_{m=1}^{N_B} \sum_{s=1}^{N_L} \Phi_s(r_m) \exp(i k_m \cdot R_s) \right] .$$

(5)

This expansion is analogous to an inverse Fourier transform, giving a particle-like representation of the BBC.

Equation (5) is made up of many terms. Each term consists of a product of N_B factors, each of the form $\Phi_s(r_m) \times \exp(i k_m \cdot R_s)$. In each product, the deuteron index m never repeats, but the unit cell index s may repeat. In the bracketed portion of Eq. (5), when the phase factor is neglected, there are subsets of terms containing multiple values of m contributing to specific fixed site s Wannier functions $\Phi_s(r_m)$. All terms for which n values of m contribute to any of the $\Phi_s(r_m)$ correspond to n-fold occupation of the lattice site s. For large N_B, small c, and small occupation number n, there are $(N_L)^{N_B} c^n / n!$ terms corresponding to n-fold occupations by distinguishable bosons. In the evaluation of transition matrix elements in which the initial state is formed from indistinguishable bosons, these n-fold occupation terms become $n!$ degenerate because of the equivalence of $n!$ permutations of the coordinate dependencies in each of these terms. Thus, there are $(N_L)^{N_B} c^n$ terms corresponding to n-fold occupations by indistinguishable bosons.

In the next section, we are concerned with double occupations, which we call di-deuterons. Ignoring normalization and phase factors and using the wave function form of Eq. (3), the terms that describe a di-deuteron in unit cell 61 are all of the form

$$\exp\left[\frac{-3(r_{38} - R_{61})^2}{2a^2} \right] \exp\left[\frac{-3(r_{412} - R_{61})^2}{2a^2} \right]$$

$$\times \prod_{m=1, s(m) \neq 61}^{N_B - 2} \Phi_{s(m)}(r_m) .$$

A key point is that the wave functions describing this di-deuteron are all centered on the same point, R_{61}. In other words, the algebra of the many-body wave function, not tunneling, provides the overlap needed for nuclear interaction.

COALESCENCE FLUCTUATIONS

Consider the properties of band-state D^+ (i.e., of a D^+ BBC) and the resulting nuclear interactions that are implied by self-interaction. As discussed later, the magnitude of the electrostatic self-interaction V^{elec} is reduced dramatically within a solid. Nuclear self-interaction provides the dominant, nonnumber-conserving form of interaction, and, before and in the presence of self-interaction, there is an uncoupling of the motion of the center of mass (r_{cm}) from variations in the proton-neutron separation (r_{n-p}) in each single-particle D^+ wave function Φ_{deut}, through the Born-Oppenheimer separability condition:

$$\Phi_{deut} = \Phi^{elec}(r_{cm}) \Phi^{nuc}(r_{n-p}) .$$

Here, $\Phi^{elec}(\boldsymbol{r}_{cm})$ varies on the length scale of the electrostatic interaction, while $\Phi^{nuc}(\boldsymbol{r}_{n\text{-}p})$ varies over the range of the strong interaction. The band-state D^+ initial state becomes occupied when sufficient numbers of D^+ ions become indistinguishable on the length scale of the electrostatic interaction and the associated single-particle wave functions $\Phi^{elec}(\boldsymbol{r}_{cm})$ approach the single-particle ψ_{Bloch} states of Eq. (2). Equation (5), then, describes the many-body electrostatic wave function, with the understanding that each Wannier state $\Phi_s(\boldsymbol{r}_m)$ is multiplied by a site-independent nuclear wave function Φ^{nuc}, which depends only on the value of $\boldsymbol{r}_{n\text{-}p}$ and not on the location within the lattice of the deuteron. Bounds on the rate of nuclear self-interaction can be obtained from the absolute square of the integral of the multiply occupied initial-state product, $\Phi_s(\boldsymbol{r}_1), \ldots, \Phi_s(\boldsymbol{r}_{N_B})$, multiplied by a more compactly distributed product of final-state wave functions in which all of the final electrostatic deuteron functions fall within the nuclear force range $\boldsymbol{r}_{nuc}$. This particle-like interaction is a coalescence fluctuation in which two initial-state Wannier functions coalesce over a volume $\upsilon_{nuc} = 4\pi r_{He}^3/3$. Here the nuclear interaction radius is chosen to be equal to the radius of the $^4\mathrm{He}$ nucleus r_{He} ($= \sim 2 \times 10^{-13}$ cm). These coalescence fluctuations provide a channel for forming a four-fermion "nuclear bag" state analogous to a free-space $^4\mathrm{He}$ nucleus:

$$\Phi_s(2,\boldsymbol{r})_{Bloch} \rightleftarrows \Theta_s(2,\boldsymbol{r}_{\mathrm{He}})_{Bloch} \ , \tag{6}$$

where $\Phi_s(2,\boldsymbol{r})_{Bloch}$ is the set of terms describing a double occupation of unit cell s. Each set of terms $\Phi_s(2,\boldsymbol{r})_{Bloch}$ represents a di-deuteron and $\Theta_s(2,\boldsymbol{r}_{\mathrm{He}})$ represents the nuclear bag-like configuration. This fluctuation may be viewed as the particle-like representation of the band-state fusion reaction

$$2D^+{}_{Bloch} \rightleftarrows {}^4\mathrm{He}^{++}{}_{Bloch} \ . \tag{7}$$

FUSION REACTION RATE

We calculate the coalescence fluctuation rate per di-deuteron N in the presence of a $^4\mathrm{He}^{++}$ BBC from the Fermi Golden Rule[16]:

$$\dot{N} = 2\pi/\hbar \sum \langle i|V|f\rangle \langle f|V|i\rangle \delta\left(E_i - E_f\right) . \tag{8}$$

Here

$$|i\rangle = \Psi_D\left(\varepsilon_m, r\right) \cdot \Psi_{He}\left(\varepsilon_\rho, r\right)$$

Where $\psi_D(\varepsilon_p, r)$ denotes the initial D^+ BBC state of Eq. (5), and the balance of the equation represents the initial $^4\mathrm{He}^{++}$ BBC state. Also, $\delta(E_i - E_f)$ is the delta function in which E_i is the initial total energy and E_f is the final energy. The delta function guarantees conservation of energy between initial and final states. The V operator preserves Born-Oppenheimer separability, thereby eliminating all but those interactions that preserve tightly bound neutron-proton pairs, leading to a bosons in/bosons out selection rule.[5,8] Only the terms of Eq. (6) give nonzero values to the di-deuteron overlap integral.

Equation (8) can be evaluated using either the Wannier or the Bloch state representation of the wave functions. Because we are concerned with interaction between distributed states, we choose to work with Bloch states. The final state is the product of a D^+ band state decremented by two D^+ and a $^4He^{++}$ band state augmented by one $^4He^{++}$:

$$|f\rangle = [1/(N_D-2)!]^{1/2} \sum_{\{r_m\}} \prod_{m=1}^{m'-1} \prod_{m=m'+1}^{m''-1} \prod_{m=m''-1}^{N_D} \psi_D(k_m, r_m)$$
$$\times (1/N_D)^{1/2}[1/(N_D-1)]^{1/2}[1/(N_{He}+1)!]^{1/2}$$
$$\times \sum_{\{r_p\}} \psi_{k_1+k_2}[(r_{m'}+r_{m''})/2]\Phi^{nuc}(r_{m'}-r_{m''})$$
$$\times \prod_{p=1}^{N_{He}} \psi_{He}(k_p, r_p) \ .$$

(9)

Here $(r_{m'} + r_{m''})/2$ is to be included as an additional coordinate in the symmetrizing summation over $\{r_p\}$, and $\Phi^{nuc}(r_{m'} - r_{m''})$ is a compact nuclear function that is appreciable only when $|r_{m'} - r_{m''}| < R_{He} = \sim 2 \times 10^{-13}$ cm, where R_{He} is the effective radius of a $^4He^{++}$ nucleus. In the overlap with the initial state, $N_D(N_D - 1)$ terms from the sum of products in the initial state contribute coordinates $r_{m'}$ and $r_{m''}$. When each contribution from the deuteron band population associated with the coordinates $r_{m'}$ and $r_{m''}$ is re-expressed in terms of $(r_{m'} + r_{m''})/2$ and the symmetrization sum over $\{r_p\}$ is carried out, $N_{He} + 1$ equivalent contributions are obtained.

To establish a lower bound on the D^+ BBC concentration required for the observed heating,[2] we assume that each coalescence fluctuation leads to occupation of the $^4He^{++}{}_{Bloch}$ state, i.e., the creation of an additional member of the $^4He^{++}$ band-state population. In this process, it is required that $\psi_{k_1+k_2}[(r_{m'}+r_{m''})/2]$ has perfect overlap with the comparable contribution associated with the center-of-mass motion of the di-deuteron fluctuation. Consistent with this approximation, we treat the square-well self-interaction nuclear potential case, in which an isolated square well is defined by an upward shift in kinetic energy T_0 of each D^+ ion over the characteristic nuclear dimension r_{nuc} near each of the periodically equivalent $(r_{m'} + r_{m''})/2$ locations where fusion occurs. We assume that the nuclear potential is nonvanishing only when the overlapping deuterons have opposed spins. The energy release per reaction V_0 is 23.8 MeV. Because the energy release is distributed over all unit cells, the magnitude of the shift in kinetic energy is 23.8 MeV/N_L at each lattice site. The volume of each of the N_L potential wells is v_{nuc}. Consistent with these approximations, we replace the four-body nucleon problem associated with the two neutron-proton pair functions with a single-body problem in which the two initial- and final-state electrostatic functions are replaced by a single initial- and final-state wave packet, whose characteristic size is determined by the characteristic length scale of the center-of-mass motion of initial and final states. This is equivalent to a localized reaction in which all nuclear energy is transiently transferred directly into deuteron motion and treating all nucleons with an independent nucleon model. Also, consistent with this choice of model, the final density of states $\rho(E) = dn/dE$ is

$$\rho_f(0) = 1/(\hbar\omega_{nuc}) \ ,$$

where $\omega_{nuc} = (3\hbar/2)(m_B r_{He}^2)$, and $E = \sim 0$ is the energy level of the BBC D^+ and $^4He^{++}$ bands in the lattice. For simplicity, we consider the low-temperature limit. This allows us to choose vanishing values for all wave vectors k_m in Eq. (5). Because $\psi_{k_1+k_2}[(r_{m'} + r_{m''})/2]$ has perfect overlap with the comparable initial-state contribution associated with the dependence of $\psi_{k_1}(r_{m'})\psi_{k_2}(r_{m''})$ on $(r_{m'} + r_{m''})/2$, it follows that the only remaining nontrivial contributions to the matrix element involve the integral of an initial wave function $\psi_{packet,i}$ having a characteristic dimension of electrostatic zero-point-motion size multiplied by a function $\psi_{packet,f}$ nuclear size. Thus, for initial and final states, we may use wave packet forms,

$$\psi_{packet,i} = [2/(\pi\alpha^2)]^{3/4} \exp(-r^2/\alpha^2)$$

and

$$\psi_{packet,f} = [3/(2\pi r_{He}^2)]^{3/4} \exp(-3r^2/4r_{He}^2) \, ,$$

to compute this integral. The overlap integral O(J) is

$$O(J) = (16/3)^{3/4} \ (v_{nuc}/v_{har})^{1/2} \quad .$$

The volumetric reaction rate $\dot{n}$ is

$$\dot{n} = (16/3)^{3/2} \ [2\pi V_O^2/\hbar] \ [v_{nuc}/v_{har}]$$
$$[2m_B R_{nuc}^2/(3\hbar^2)] \ [c_D^2 c_{He}/v_{site}] \, . \tag{10}$$

Here v_{site} is the unit cell volume of PdD, and $v_{har} = 4\pi/3 \ a^3 = 7.76 \times 10^{-26} \ cm^3$ is the zero-point-motion volume defined by Eq. 3. Using the heat release associated with reaction (7) for the magnitude of the perturbation $V_O = 23.8$ MeV, and assuming that averaging over the initial spin reduces the rates by a factor of 1/3, we obtain a lower bound for $c_D = c$

$= 4.3 \times 10^{-11}/c_{He}^{1/2}$ for a volumetric power density[2] $\dot{n} \ V_O = 600$ W/cm^3.

An important consequence of Eq. (10) is that the reaction rate for the decay of a single pair of BBC deuterons from the D^+ band state to the $^4He^{++}$ band state is proportional to c_{He}. This means that band-state $^4He^{++}$ can help to promote nuclear reaction. This possibility may provide an explanation for the observation that pretreatment of the electrodes with helium seems[10] to increase the probability for heat production.

ELECTROSTATIC SELF-INTERACTION

The BBC picture presented here uses single-particle wave functions that have no explicit electrostatic ion-ion correlation terms because *such wave functions minimize total ground-state energy subject to the constraints imposed by particle statistics and symmetry.* Nonetheless, inclusion of the D^+-D^+ electrostatic interaction affects the BBC by introducing a many-body interaction that could affect the band picture from which the BBC is derived. The band picture remains valid provided that each D^+ remains well screened in the initial state and in the presence of self-interaction. Satisfactory screening occurs provided the BBC concentration is sufficiently

low. A breakdown of the application of the band picture for describing nuclear behavior occurs when the time scale associated with electrostatic self-interaction for multiply occupied Wannier states becomes comparable to the wave function oscillation period within the nuclear potential well τ^{nuc}. The difference between τ^{elec} and τ^{nuc} determines whether or not the electrostatic and nuclear interactions are separable and thereby determines the appropriateness of the form assumed for each mutually noninteracting boson wave function in the nuclear reaction calculation.

Each n-fold occupation component of the BBC has particle character when it is expressed as a virtual state described by Wannier functions. The virtual states describe a transient occupation of a unit cell by an integer number of deuterons. The lifetime of the n-fold multiple occupation virtual state is determined by the self-interaction energy ΔE_n, except for the single-occupation state. Since the BBC is in thermodynamic equilibrium with non-BBC deuterium, ΔE_1 must be small; otherwise, BBC states would not be occupied. The term ΔE_2 is the difference in self-interaction between single and double occupation of a unit cell and can be estimated using the Wannier state wave functions defined by Eq. (3):

$$\Delta E_2 = \frac{3}{2} \int e^2 f(r) f(r') / |r - r'| \, dr \, dr' \, , \tag{11}$$

where $f(r) = [\Phi(r)]^2$ and e is the electron charge. Using a realistic value[12] for a (= 0.5 Bohr), we find $\Delta E_2 = 81.6$ eV. (This is the value previously used in the calculation of the relative stability of the D^+ band-state matter configuration.) The corresponding Planck lifetime $\tau^{elec2} = h/\Delta E_2$ is $\tau^{elec2} = 5.1 \times 10^{-17}$ s. This electrostatic Planck time compares with the nuclear Planck time $\tau^{nuc} = h/V_0 \sim 10^{-22}$ s. This large difference justifies the Born-Oppenheimer separable form for Φ_d used in the last section, which leads to an uncoupling of the nuclear and electrostatic degrees of freedom. Thus, zero-point motion reduces $\Delta E_{electrostatic}$ by five orders of magnitude from its free-space value, which is comparable to ΔE_{nuc}. If it were not for the dominance of the lattice interaction, the free-space electrostatic interaction energy would apply, Born-Oppenheimer separability would not apply, and fusion would be prevented.

ESTIMATE OF ION BAND-STATE CONCENTRATION FOR Pd-D COLD FUSION

The physical picture presented seems an adequate description for fusion in AgD_δ. It may need modification for $PdD_{1+\delta}$ to take into account the Coulomb repulsion of the chemically bonded deuterium atom that occupies each unit cell. In general, the expectation is that, at low band-state concentration, both the octahedral symmetry of the stoichiometric PdD lattice and the spatial density distribution of the chemically bonded deuterium is unaffected by deuterium addition. The band-state D^+ shares the octahedral site with the chemically bonded deuterium. A concentration-dependent dilation of the lattice with deuterium addition is to be expected.

On the other hand, our use of a harmonic well for the single-particle potential seen by the band-state D^+ approximated from the well associated with the known zero-point motion of the chemically bonded deuterium could be an oversimplification. Anharmonic effects can enter the band-state D^+ potential through (a) the repulsion that the band-state deuterons experience as a result of interaction with chemically bonded deuterium located at the octahedral sites and (b) ef-fects due to coupling with the itinerant electrons. When the zero-point motion of chemically bonded deuterium is sufficiently large or the zero-point-motion volume is approximately neutral,

our use of this harmonic approximation should be adequate. When the zero-point volume of the chemically bonded deuterium is not fully neutralized, an anharmonic potential may apply, and the ground-state wave function of the added deuterons becomes more complicated. In this case, however, an "effective" harmonic model, involving an enlarged zero-point motion, may be used to estimate the effects of concentration on cold fusion. In any case, υ_{har} cannot be larger than υ_{site}.

The reaction rate given in Eq. (10) is considered an upper limit because of three factors: (a) our use of υ_{har} based on observations of chemically bonded deuterium for the effective volume of $\Phi_s(\boldsymbol{r})$, (b) the inclusion of spin as the only nuclear inhibiting factor affecting reaction, and (c) the neglect of the inverse reactions implicit in the reversible coalescence fluctuation picture. This technical note does not resolve these uncertainties. We conservatively estimate the perfect lattice $PdD_{1+\delta}$ reaction rate as follows: If we assume an upper limit for $\upsilon_{har} = \upsilon_{site}$, the lower bound concentration for 600 W/cm^3 power density (c_{600}) is increased by a factor of 13.8, giving $c_{600} = 5.9 \times 10^{-10} / c_{He}^{1/2}$. With respect to nuclear inhibiting effects, we know of no intrinsic nuclear factors other than spin that will reduce the reaction rate. To understand the implication of inverse reactions, we may estimate the relative rates for the reversible fluctuations and the thermal effects which inhibit reversibility. For a 0.1-mm crystal containing 10^9 D$^+$ band-state ions and a power density of 600 W/cm^3, we calculate a reaction rate $\dot{n} = 1.6 \times 10^{14}$ fusion/s-cm^3. This corresponds to a crystal reaction rate $\dot{N} = 1.6 \times 10^8$ fusion/s. The corresponding reaction time is $\tau_{fuse} = 6 \times 10^{-9}$ s. At room temperature, we envision symmetry-breaking interactions (such as through phonons, thermal damage, etc.) with the lattice using an interaction energy of $\Delta E_{SB} = k_B T = 0.025$ eV, with corresponding symmetry-breaking time $\tau_{SB} = h/\Delta E_{SB} = 1.7 \times 10^{-13}$ s. Since the time for energy transfers to the lattice from energized band-state ions is very much less than τ_{fuse}, the symmetry-breaking interactions with the lattice should prevent coalescence reversal. We conclude that, at the low concentrations involved, each coalescence fluctuation is equivalent to a reaction.

SUMMARY

We have postulated a new form of matter, namely, ion band-state matter within a metallic host solid. This type of matter can form when low concentrations of deuterium, helium, and possibly other light atoms are embedded as low-concentration impurities in a suitable metallic host. In the ion band-state configuration, the ions derived from these atoms assume a delocalized, standing wavelike distribution, while the neutralizing electrons occupy a portion of the host's conduction electron population. An electrostatically stable ion band-state matter component forms if and only if the host + impurity system has a lower chemical potential with the distributed matter form than it has with a sparse, squeezed molecule population of discrete interstitial chemical occupations of scattered unit cells. The ion band-state configuration avoids the endothermic localized lattice strain term in the chemical potential but requires an endothermic ion-ion Coulombic repulsion term. The repulsion term is a result of multiple occupations of unit cells implicit in the many-body wave function description of bosonic band states. The Coulombic repulsion term is concentration dependent and vanishes in the low-concentration limit. For this reason, ion band-state matter should be the stable matter form at very low concentration.

Ion band-state matter differs from chemical matter in its quantum-mechanical description because, in band-state matter, the dominant interaction is the electrostatic interaction with the

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lattice. All other interactions are perturbations to this dominant interaction. The single-particle wave functions contain no explicit band-state-ion/band-state-ion interaction terms because without such terms the many-body wave function provides a minimum energy configuration of the total system. With chemical matter, all Coulombic interactions are explicit. The mass density of solids is determined by the relatively large deBroglie wavelength of the electron. When such structures are composed only of chemical matter, the core ion-ion Coulomb repulsion terms prevent nuclear wave function overlap. In contrast, for bosonic band-state matter, the algebra of the many-body wave function dictates wave function overlap. For a mix of D^+ and $^4He^{++}$ band-state matter, the resulting D^+-D^+ overlap with $^4He^{++}$ leads to augmentation of band-state $^4He^{++}$ with an ultimate increase in system entropy at the expense of nuclear potential energy. This is the basis for the cold fusion heat effect.

At sufficiently low temperature, the greatest overlap between initial and final states occurs when the final-state $^4He^{++}$ remains primarily ionically bound within the periodic (bulk) lattice and when energy release to the environment does not result from processes that destroy the periodic symmetry associated with either the final or the initial state. As a consequence, it is to be expected that ^4He will predominantly remain untrapped and in an ionic form within each solid crystalite and will be distributed uniformly therein. Thus, the model predicts (in agreement with experiment[5-10]) that atomic (i.e., neutral) ^4He will primarily be found either in the surface regions, near interfaces and impurities, or in the outgases, where periodic order is disrupted, and not within the interior of the bulk solid crystals.

IMPLICATIONS FOR EXPERIMENTS

Lack of reproducibility is still encountered in many cold fusion experiments. In palladium, this lack of reproducibility is likely due to the difficulty of maintaining the nonequilibrium concentration of deuterium in PdD_x required for D^+ band-state formation. In a stoichiometric PdD host, to provide the concentration electrochemically, electrode surfaces must not catalyze the $D + D \rightarrow D_2$ reaction. Control of this surface catalysis is notoriously difficult.

However, another factor may be equally important. The presence of a nonnegligible concentration of band-state $^4He^{++}$ is required for the two-band-state reaction described here. Although alternative reaction channels for cold fusion with lower probability exist, in which the $^4He^{++}$ band is initially unoccupied, the D^+ to $^4He^{++}$ band-state reaction could be the most important one. As previously noted, there is evidence that ^4He impregnation seems to enhance the probability for reaction. It is also clear from theory that ^4He probably will be expelled away from the bulk crystals. Proper monitoring of outgases for ^4He is an important experimental procedure. This kind of procedure has not yet been adequately carried out in any cold fusion experiment.

A variety of additional cold fusion-related phenomena have been reported by various observers. Some of these have been interpreted in the context of our theory. These interpretations are given in Ref. 8.

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