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Nuclear Fusion in a Solid via a Bose Bloch Condensate

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We present a theory of solid state fusion based on the formation of a D^+ bosonic Bloch condensate within a metal deuteride. The first step towards fusion is a coalescence reaction which converts a 4-fold occupation state of zero point motion size into a state of nuclear dimensions. Reaction rates for the coalescence reaction are calculated using the Fermi Golden Rule.

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CONTENTS

NUCLEAR FUSION IN A *SOLID* VIA A *BOSE BLOCH CONDENSATE*

Introduction

This paper discusses a concept of solid state fusion based on the formation of a D^+ boson Bloch condensate (BBC)[1] within a palladium deuteride host lattice. Evidence for such solid state fusion has been presented by Fleischmann and Pons[2], who have described episodic generation of anomalous heat in Pd cathodes following extended overvoltage electrolysis of LiOD solutions. Other evidence for solid state nuclear interactions in PdD_x includes the observations of surface hydrogen isotopic anomalies in Pd cathodes subsequent to such electrolysis[3,4] and the possible observation of a small number of 20+ Mev energy release events in a Si charged-particle detector adjacent to a Pd electrode charged with D^+ ions by ion implantation[5].

The bosonic Bloch condensate

The D^+ BBC is a collective bosonic condensate derived from weakly bound D^+ ions which are well-screened but constrained to an approximately periodic arrangement through electrostatic interaction with a host lattice. The resulting Bloch symmetry permits the condensate to exist at low boson concentration $c = N_B/N_L$, where N_B is the number of condensate bosons and N_L is the number of unit cells in the host crystal. The BBC is a collective, cooperative entity which contributes fractional charge per unit cell. It undergoes integer occupation fluctuations at individual sites, expressed by Wannier functions.

Palladium hydride and conditions favoring D^+ BBC formation

The PdH_x and PdD_x systems have been studied extensively[6]. PdD_x differs from PdH_x by having a lower equilibrium pressure at any given x. Both materials are superconducting at low temperature with PdD_x having a higher transition temperature. This higher transition temperature, and the higher diffusivity of D as opposed to H in Pd are contrary to expectations based on increased mass. Absorption of D into PdD_x expands the lattice and causes local strain when x is small. This strain energy is

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a component of the chemical potential, which is very positive at low x, becoming very negative as x→1. As x→1, D additions remove local strain due to isolated vacancies. This x-behavior of the chemical potential suggests that values of x very near x=1 should be favorable for formation of a D^+ BBC. Very near x=1, the limited availability of vacancies dictates that some unit cells will contain more that 1 D^+ ion. Without formation of a D^+ BBC, these sites must be doubly occupied, creating high local lattice strain, hence a high positive chemical potential. When a D^+ BBC forms, the excess D^+ charge is shared by all periodically equivalent sites in the crystal, avoiding local lattice strain. Hence the D^+ BBC should be thermodynamically favored.

D^+ BBC fusion reactions

Nuclear reactions from a D^+ BBC state in a crystal lattice are possible because, from such an initial state, the electrostatic barrier problem of free space nuclear interaction may be eliminated. Fusion is a result of three D^+ BBC properties: screening by the lattice for $c << 1$, the resulting large zero point motions associated with this screening, and the multiple boson occupation of single lattice sites. (Here BBC-D^+ refers to the D^+ ions that have become part of the BBC, and does not include D^+ ions which are part of the host lattice. Henceforth D^+ shall refer to BBC-D^+ unless otherwise indicated.) The large zero point motion spreads out the D^+ charge density within a unit cell. The resultant reduction in the self-interaction associated with multiple occupation virtual states increases the time constant for electrostatic interaction relative to that for nuclear interaction, leading to a separability of interaction modes, as discussed further below. Since each D^+ BBC ion "sees" an approximately periodic potential, the single particle density at a given site is derived from a superposition of different Bloch symmetric eigenstates. The associated density at a given site can be viewed as either a superposition of non-stationary, Wannier state densities, each of which is localized primarily

around an individual site, or as a superposition of time independent Bloch state densities, each of which extends throughout the lattice. In the evaluation of the transition matrix element associated with fusion, the initial state wave functions and fusion-inducing changes in the potential result from non-number conserving, many-body fluctuations associated with multiple occupation of Wannier states at a given site. Site multiple occupation causes deuteron wave functions to overlap, inducing fusion.

BBC formation using bosons which interact only with the lattice

We first consider a BBC formed from mutually-non-interacting bosons. These bosons interact only with a host metal lattice and its itinerant electron population. Boson-boson interactions are ignored.

We consider the case of the N_B bosons 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 $\psi_{Bloch}(\mathbf{k},\mathbf{r})$ for the ideal lattice have the property

$$\psi_{Bloch}(\mathbf{k},\mathbf{r}+\mathbf{R}) = \psi_{Bloch}(\mathbf{k},\mathbf{r})\ \exp(i\mathbf{k}\cdot\mathbf{R}) \quad . \quad (1)$$

The fluctuation properties are shown by expanding in terms of Wannier functions

$$\psi_{Bloch}(\mathbf{k},\mathbf{r})\ \exp(-\epsilon(\mathbf{k})t/\hbar) = (1/N_L)^{1/2} \sum_{s=1}^{N_L} \phi_s(\mathbf{r},t)\ \exp(i\mathbf{k}\cdot\mathbf{R}_s) \ , \quad (2)$$

where $\mathbf{R}$ and $\mathbf{R}_s$ are Bravais lattice vectors, $\epsilon(\mathbf{k})$ is the band energy of ψ_{Bloch}, and $\mathbf{k}$ is the crystal momentum. Each ϕ_s is a Wannier state, which, in the harmonic approximation, is suitably approximated at t=0 by the ground state wave function of a

parabolic well,

$$\phi_s(\mathbf{r}) = (2/\pi a^2)^{3/4} \exp(-\mathbf{r}_s^2/a^2) \quad , \qquad (3)$$

where $\mathbf{r}_s = \mathbf{r}-\mathbf{R}_s$, and a is the classical turning point of the well.

The many body wave function associated with the occupation of N_B band states (denoted by eigenvalues ϵ_p) possessing N_B coordinate dependencies $\mathbf{r}$ is given by

$$\Psi(\epsilon_p,\mathbf{r}) = (1/N_B!)^{1/2} \sum_{\{\mathbf{r}_m\}} \prod_{m=1}^{N_B} \psi_{Bloch}(\mathbf{k}_p,\mathbf{r}_m) \quad , \qquad (4)$$

where 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. Substituting Eq. 2 into Eq. 4, we find that

$$\Psi(\epsilon_p,\mathbf{r}) = (1/N_B!)^{1/2} \sum_{\{\mathbf{r}_m\}} (1/N_L)^{N_B/2} \left(\prod_{m=1}^{N_B} \sum_{s=1}^{N_L} \phi_s(\mathbf{r}_m) \exp(i\mathbf{k}_p\cdot\mathbf{R}_s) \right) . \qquad (5)$$

In the bracketed product of summed terms in Eq. 5 there exist subsets of terms containing multiple values of m contributing to fixed site s Wannier functions $\phi_s(\mathbf{r}_m)$. All terms for which n values of m contribute to any of the $\phi_s(\mathbf{r}_m)$ correspond to n-fold occupation of the lattice site s. For large N_B, small c, and small occupation number n there exist $(N_L)^{NB}\ c^n/n!$ terms corresponding to n-fold occupations by distinguishable bosons. For indistinguishable bosons, these terms become n!-degenerate due to the equivalence of n! permutations of the coordinate dependencies in each of these terms. Thus there are $(N_L)^{NB}\ c^n$ terms corresponding to n-fold occupations by indistinguishable bosons. For notational purposes, we regroup terms in Eq. 5 that

correspond to different n-fold occupations. The corresponding collection of terms we designate as $\phi(n,k_p,r)$. Thus

$$\Psi(\epsilon_p,r) = \sum_{n=1}^{N_B} \phi(n,k_p,r) \quad .$$

In the next section we will be concerned with 4-fold occupations, which we call quad-bosons.

Nuclear reactions

We now consider the properties of D^+ BBC bosons and the resulting nuclear interactions that are implied by self-interaction. As discussed in the next section, the magnitude of the electrostatic self-interaction V^{elec} is reduced dramatically within a solid. As a consequence, nuclear self-interaction provides the dominant, non-number conserving form of interaction at one or a set of lattice sites. A further consequence of the reduction of V^{elec} involves 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 ψ_{deut} through the separability condition,

$$\psi_{deut} = \psi_{elec}(r_{cm}) \quad \psi_{nuc}(r_{n-p}) \quad .$$

Here, $\psi_{elec}(r_{cm})$ varies on the length scale of the electrostatic interaction, while the spatial variation of $\psi_{nuc}(r_{n-p})$ occurs over the range of the strong interaction. The initial state D^+ BBC component 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 $\psi_{elec}(r_{cm})$ approach the single particle ψ_{Bloch} states of Eq. 2. Eq. 5, then, may be used to describe the many-body electrostatic wave function for the D^+ BBC initial state, with the understanding that each Wannier state $\phi_s(r_m)$ is multiplied by a site independent nuclear wave function ψ_{nuc}, which depends only on the value of r_{n-p} and not on the location within the lattice of the deuteron. Bounds on the probability of nuclear self-interaction then can be

obtained from the absolute square of the integral of the multiply occupied initial state product, $\phi_s(r_1) \ldots . \phi_s(r_n)$, multiplied by a more compactly distributed product of final state wave functions in which all of the final electrostatic boson functions fall within the nuclear force range r_{nuc}. From the "bosons in and bosons out" selection rule of ref. 1, we are led to explore a reaction in which four initial state Wannier functions coalesce over a volume $V_{nuc} = 4/3\ \pi\ r_{nuc}^3$, forming an eight fermion "nuclear bag" state analogous to a free space excited $^8Be^*$ nucleus. Symbolically we will refer to this coalescence reaction as

$$\phi(4,k_p,r) \rightarrow \theta(4,k_p,r_{nuc})_{Bloch} \quad , \qquad (6)$$

where $\theta(4,k_p,r_{nuc})$ represents the "nuclear bag-like" configuration. This reaction is the first step in the fusion reaction

$$4D^+_{Bloch} \rightarrow {}^8Be^*_{Bloch} \rightarrow 2\ {}^4He \quad . \qquad (7)$$

We calculate the reaction rate from the Fermi Golden Rule[7],

$$\dot{n} = 2\pi/\hbar \ \Sigma\ \langle i|V|f\rangle \langle f|V|i\rangle\ \delta(E_i - E_f) \quad , \qquad (8)$$

where $|i\rangle$ denotes this inital D^+ BBC state. The sum is over final states $|f\rangle$, where

$$|f\rangle = (1/N_B!)^{1/2} \sum_{\{r_m\}} \prod_{m=5}^{N_B} (1/N_L)^{N_B/2} \sum_{s=1}^{N_L} \phi_s(r_m)\ \exp(ik_p \cdot R_s) \cdot \phi_d(r_1)\phi_d(r_2)\phi_d(r_3)\phi_d(r_4) \qquad (9)$$

where ϕ_d is a compact "defect" function, centered at the single site r_{fusion} where fusion takes place and has spatial variation in its center of mass coordinate only over the range r_{nuc}. Also $\hbar = h/(2\pi)$, where h is the Planck constant, and $\delta(E_i - E_f)$ is the δ-

function in which E_i is the initial total energy and E_f is the final energy. The δ-function guarantees conservation of energy between initial and final states. The operator V refers to the nuclear self-interaction potential.

To establish a lower bound on the required BBC concentration associated with the observed heating[2], 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_o of each D^+ ion over the characteristic nuclear dimension r_{nuc} near r_{fusion}. The volume of the well is derived from $r_{nuc} = 9.1 \times 10^{-13}$ cm, appropriate for a mass 8 nucleus. This is equivalent to immediate dissipation of α-particle product energy in the reversed reaction within the region where interaction takes place. Consistent with these approximations we replace the eight body nucleon problem associated with the four defect functions with a single body problem in which the four 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 transfering all nuclear energy directly into alpha particle 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 $\omega_{nuc} = (3\hbar/2) /(m_B R_{nuc}^2)$, m_B is the deuteron mass, and $E = \sim 0$ is the energy level of the BBC deuteron band in the lattice. We choose vanishing values for all wave-vectors k_p in Eq. 5 since the case of an isolated perturbation applies to low temperature. For initial and final states, we use wave packet forms

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

$$\psi_{packet,f} = (3/(2\pi R_{nuc}^2))^{3/4} \exp(-3r^2/4R_{nuc}^2) \quad ,$$

where r is measured from the center of boson mass in each unit cell and $R_{nuc} = (3/4\pi \ V_{nuc})^{1/3}$. The overlap integral O(J) is

$$O(J) = (16/3)^{3/4} \ (V_{nuc}/V_{bar})^{1/2}$$

and

$$\dot{n} = (16/3)^{3/2} \ 2\pi V_o^2/\hbar \ 2m_B R_{nuc}^2/(3\hbar^2) \ V_{nuc}/V_{bar} \ c^4 \ . \qquad (10)$$

In the calculation O(J) receives contributions from each unit cell in the crystal. Using the heat release associated with reaction (7) for the magnitude of the perturbation V_o = 47.6 MeV, we obtain a lower bound for $c = 2.8 \times 10^{-7}$ for a volumetric power density output $\dot{n}V_o/V_{site} = 10$ W/cm^3, as observed in ref (2). (V_{site} is the unit cell volume of Pd.)

Electrostatic self-interaction (the coulomb barrier)

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^+ (within or outside the BBC) remains well-screened. However, a breakdown of the application of the band picture for describing nuclear behavior occurs when the timescale τ^{elec} associated with electrostatic self-interaction for multiply occupied Wannier states becomes comparable to the timescale associated with nuclear self-interaction τ^{nuc}. The difference between τ^{elec} and τ^{nuc} (= the inverse of the nuclear reaction rate) determines whether or not the electrostatic and nuclear interactions are separable, and thereby determines the appropriateness of the form assumed for each mutually-non-interacting boson wave function in the nuclear reaction calculation, described in the last section.

Each n-fold occupation component of the BBC is a single entity whose particle character is evident only through the existence of virtual states as described by the 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 in the lattice, ΔE_1 must be small, otherwise BBC states would not be occupied. ΔE_2 is the difference in self interaction between single and double occupation of a unit cell, and can be evaluated using the Wannier state wave functions defined by Eq. 3:

$$\Delta E_2 = 3/2\ e^2 \int\int \frac{|\phi_s(r)|^2\ |\phi_s(r')|^2}{|r-r'|}\ d^3r\ d^3r' \quad . \qquad (11)$$

Using a = 0.5 Bohr, we find ΔE_2 = 81.6 eV. Similarly ΔE_4 = 408 eV. The corresponding Planck lifetimes $\tau^{elec}_n = h/\Delta E_n$ are τ^{elec}_2 = 5.1 x 10^{-17} s and τ^{elec}_4 = 1.0 x 10^{-17} s. These electrostatically determined lifetimes compare with the Planck time $\tau^{nuc}_4 = h/V_o$ ~ 10^{-22} s, associated with self-induced nuclear interaction that results from quadruple occupation (as modeled by four distinguishable single particle deuteron wave functions which coalesce within a common nuclear volume). The large difference in electrostatic and nuclear lifetimes justifies the Born-Oppenheimer separable form for ψ_{deut} used in the last section, which leads to an uncoupling of the nuclear and electrostatic degrees of freedom. The reduction in charge density caused by D^+ harmonic motion inside the unit cell thus 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 lattice interaction, the free space interaction energy would apply, Born-Oppenheimer separability would not apply, and fusion would be prevented.

D^+ BBC Interactions in PdD

The last section describes a D^+ BBC volumetric nuclear self-interaction that is calculable using the Bloch eigenstates of the system and that approximately conserves crystal momentum. The reactions do not refer to any particular value of x. However, the most favorable condition for D^+ BBC formation is $x \to 1$. Under these conditions interaction of the BBC with non-BBC D^+ may be possible. The applicable reactions would be

$$3D^+_{Bloch} \leftrightarrow {}^6Li^*_{Bloch} \qquad (12a)$$

$${}^6Li^*_{virtual} + {}^2D^+ \rightarrow {}^8Be^* \rightarrow 2 \text{ alpha} \quad . \qquad (12b)$$

The maximum rate for this reaction chain would have the same form as that of Eq. 7, but with a c^3 concentration dependence instead of a c^4 dependence, namely

$$\dot{n} = (16/3)^{3/2}\, 2\pi V_o^2/\hbar\, 2m_B R_{nuc}^2/(3\hbar^2)\; V_{nuc}/V_{bar}\; c^3 \quad . \qquad (13)$$

An alternate mode of energy release might be by successive nuclear interaction scattering reactions with non-BBC D^+. These reactions could be of the form

$$2D^+_{Bloch} \leftrightarrow {}^4He^*_{Bloch} \qquad (14a)$$

$${}^4He^*_{virtual} + D \rightarrow {}^4He^{**} + D_{scat} \qquad (14b)$$

$${}^4He^{**} + D \rightarrow {}^4He^{***} + D_{scat} \qquad (14c)$$

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

where $4He^{**}$ and $4He^{**\cdots *}$ are nuclear bag states of lower total energy than the D^+ BBC and the D_{scat} are recoil scattered non-BBC deuterons. Once reaction (14b) occurs, reaction (14a) becomes energetically blocked. Reactions (14) may be the most favorable

mode of decay. Coupling between the chemically bonded D and the lattice could result in momentum transfer to the lattice as a whole. The result could be heat release without any high energy particle generation.

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