Chubb, S.R. *Impact of Boundary Effects Involving Broken Gauge Symmetry on LENR's*. in *Tenth International Conference on Cold Fusion*. 2003. Cambridge, MA: LENR-CANR.org. This paper was presented at the 10th International Conference on Cold Fusion. It may be different from the version published by World Scientific, Inc (2003) in the official Proceedings of the conference.

Impact of Boundary Effects Involving Broken Gauge Symmetry on LENR's

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Surfaces have a huge impact on the physics and chemistry of solids. Changes in surfaces (or other boundaries of a solid), in particular, can be related to changes in the local ("chemical") environment. In the idealized limit, in which surfaces are defined as "boundaries" associated with a lack of, or accumulation of charge, dynamical effects at surfaces can be used and are required (by the associated coupling to external electromagnetic fields) to relate seemingly unrelated local and non-local effects. Thus, counter-intuitive ideas about local and non-local effects can become dominant. In particular, in PdH or PdD, provided external forces are applied uniformly, it is entirely possible for hydrogen (p) or deuterium (d) nuclei to acquire a common phase (a broken gauge symmetry[1]) and to "become wave-like" and interact coherently, through the electromagnetic field, simultaneously, but an-isotropically at the boundaries of a PdD or PdH substrate, or at isolated locations within either substrate. Also, these effects can create coupling between localized and delocalized forms of interaction. We use these and related effects as the basis for suggesting new experiments that have bearing on the findings of Iwamura et al, concerning the "apparent" transmutation of Cs to Pr.

1 Introduction

Important sources of confusion in understanding low energy nuclear reactions (LENR's) have been oversimplification, and the language associated with the underlying electrodynamics (ED), and its role in the effects. A further source of confusion has been a break down[2,3] in conventional communication about the relevant science. Mainstream ideas about the treatment of ED, and its quantum mechanical generalization (QED), as it applies in systems at room temperature (the field of many-body physics, in condensed matter systems) have been largely ignored[3]. A key point is that through wave-like effects that can occur in condensed matter systems, it is possible for large amounts of momentum to be transferred instantly in a non-local fashion. Effects related to crystalline order and related forms of symmetry can enable this to occur. As a consequence, coherent forms of interaction (that are peculiar to solids) can occur that potentially can trigger LENR's.

At surfaces or interfaces in metals, similar effects related to coherent momentum transfer can occur, but how they might relate to LENR's is counter-intuitive, i.e.: 1. Electrons (as well as p or d in ion band states[1]) can appear to become de-localized, 2. Near interfaces, electrons (or ions) can become de-localized but in a highly anisotropic manner, and 3. The charge associated with localized electrons (or ions in ion band states) can build up near an interface but be dispersed parallel to it. Thus, an-isotropic, long-range coupling can occur in which relatively large amounts of charge are found in the immediate vicinity of the interface. This can result in an effective form of trapping, in which electrons (or p or d ions) are distributed through evanescent matter wave-like states (for example), in which a relatively large accumulation of charge occurs, immediately parallel to the interface. Alternative forms of charged particle overlap can evolve from this kind of situation that may inhibit or enhance processes related to the chemisorption and adsorption of gases and related effects (including contamination/oxidation and corrosion at metallic surfaces) and the poisoning of particular catalytic reactions. Thus, for example, small quantities of metallic impurities can introduce alternative forms of de-localized interactions, resulting in longer-range magnetic or electronic coupling, potentially leading to macroscopically-large regions of ferro-magnetically active material, or to other effects involving dramatic changes in the transport of heat and electricity or optical properties in a particular material. These results can appear to be counter-intuitive because they can involve seemingly small changes in composition or small variations in externally applied forces.

In this paper, we suggest these effects could be pivotal in the Iwamura et al[4] experiments. In particular, although the 6s (valence) electrons in Cs play a dominant role in the bonding of Cs to transition metal surfaces (and in the resulting lowering of work function), more complicated effects are also important. Specifically, when Cs is adsorbed on transition metal surfaces[5,6], the (outer) 5p core electrons play a somewhat counterintuitive (but important) role in defining the associated geometry and in the resulting chemical bonds. The associated re-arrangement of charge leads to the formation of multiple, counter-polarized, electric dipoles, in which 5p core electrons, effectively, expand and contract, in response to depletion of 6s charge that results when the Cs bonds to the substrate. The resulting dipole formation is strongly correlated with depletion of charge, in and around each Cs atomic center. For this reason, it is to be expected that further polarization will take place, in response to the dissociation of D_2 gas, at the surface of the substrate, in the vicinity of each Cs. In particular, in PdD_x, with increasing x, the electronic states near the Fermi Energy are predominantly Pd-like (and have 5s, anti-bonding character). For this reason, at low Cs concentration, as D is added to PdD_x, the host material does not screen the charge of the nucleus (d) of each D appreciably, suggesting that in the experiments[4], at the Pd surface, in the immediate vicinity of the Cs, long-range, polarized forms of coupling will take place. As a consequence, the further excitation of (deeper) Cs core electrons, using X-rays (with incident energies of ~1.2 KeV), can lead to additional, significant long-range coupling through many-body ("shake-up") effects. In principle, such long-range effects could couple, non-locally, through the substrate. The associated effects may explain the significance of the CaO overlayers that are used in Iwamura et al[4] (IW). In particular, they[4] found that effects involving long-range coupling to CaO layers, in the interior of the Pd samples, appear to be playing a critical role in triggering the apparent transmutation effect.

Because of the counter-intuitive nature of a number of these effects, it is appropriate to include some background material. This is done in the next two sections. In the third section, a number of observations about the potential relevance of these effects, in the IW work, is discussed. In the final section, we suggest several new experiments.

2 Gauge Symmetry and Broken Gauge Symmetry in Wave-Like Phenomena in Condensed Matter

Wave-like phenomena, associated with broken gauge symmetry[1,7], can occur because the relationship, p=mv, between the momentum of a neutral particle and its velocity v and mass m must be modified when the particle possesses a charge e. Then the more general relationship,

$$\mathbf{mv = p - e/cA,} \quad (1)$$

applies. (A is the vector potential, and c=speed of light.)

In Eq. 1, when many charged particles acquire a common (spatially dependent) phase φ, quantum mechanically, as operators, both $\mathbf{p} \equiv \hbar / \mathbf{i} \nabla$ and e/cA can change abruptly at many different locations, instantly, without altering the value of mv. Then, many particles can respond coherently, without changing their relative positions, and velocities. The origin of this phase coherence is called spontaneously broken gauge symmetry (SBGS) [7]. SBGS can occur when many particles, instantly, become indistinguishable from each other. Then, to minimize energy, spontaneously, all particles can acquire a common phase and momentum, either in response to an outside perturbation, or to minimize energy. Well-known phenomena occur through this including: super-fluidity in liquid ^{4}He, super-conductivity, and normal heat and electrical conductivity in solids[8]. But the potential relevance of SBGS in LENR's has been ignored. Probably, this is because SBGS effects, inherently, are non-local; while nuclear reactions are local. But SBGS can explain nuclear reactions without high energy particles. In solids, SBGS occurs because of loss of translation symmetry at the boundaries of regions where charge can change in an irregular manner. To understand how this can occur, it is useful to consider a thought experiment. In figs. 1a and 1b, we show schematic diagrams of a solid and an observer, in which the observer and solid are either stationary (Fig.1a) or in motion (Fig.1b) with respect to each other. To be concrete, assume an idealized picture in which the solid is in its ground state, the observer is not interacting with it, and the motion occurs because the observer "moves" with fixed velocity V, relative to the solid. Consider the effective change in the center-of-mass (CM) wave function Ψ_{cm} of the solid that results from the change in relative motion. When both the observer and solid are stationary with respect to each other (Fig. 1a), Ψ_{cm} =1. In Fig. 1b, however, although "no interaction" occurs, in the frame of the observer,

the solid appears to "move" in a perfectly rigid fashion. Then, $\Psi(R)_{cm} = e^{i\frac{P}{\hbar}R}$, where P is the total momentum (associated with the "bulk region"[8]) of the solid (relative to the "surface region"[8]), and R is its CM. Alternatively, using the definition of the CM position, in the frame of the observer, we may re-write this last expression in the form,

$$\Psi(R)_{cm} = e^{i\frac{P}{\hbar}R} = \prod_i e^{i\frac{m(i)r(i)}{\hbar M}P} \quad .(2)$$

Here, m(i) is the mass of the i^{th} particle, and r(i) is the coordinate of its wave function.

An important point is that in the transformation that is involved with going from Fig. 1a to Fig. 1b, the many-body wave function $\Phi(r(1),.....r(n))$ associated with Fig. 1a is multiplied by the product of plane-waves that appears on the right side (R.S.) of Eq. 2. As a result, effectively, through the "rigid" (Galilean) transformation associated with going from Fig. 1a to Fig. 1b, each particle acquires a fractional portion of the total momentum, instantly.

A second important point is that the associated changes in the wave function constitute a trivial example of a gauge transformation. The transformation occurs by simply inserting a common phase factor of the form $e^{i\frac{m[i]r[i]P}{\hbar M}}$ as a prefactor of Ψ_{cm} whenever Ψ_{cm} is evaluated at the location r(i). The fact that in the absence of interacting with the solid, the observer in Fig. 1b could have chosen the relative velocity V arbitrarily means that the value of P=MV is also arbitrary. When no physically observable perturbation alters this situation, the freedom to select V constitutes a form of gauge symmetry.

Gauge symmetry of this type applies in regions that are located sufficiently far away from any boundary. Then, it is not possible to determine whether any charged "particle" is in motion or at rest, provided the charged "particle" can be identified. When no charged "particle" can be identified, the pre-factor (associated with Eq. 2) is not relevant, directly in any particular form of interaction because no net charge (or electromagnetic field) associated with any effect involving the pre-factor can be identified. However, near boundaries, or when many particles acquire a common phase, the pre-factor has important consequences. In particular, in the absence of outside forms of interaction, the energy within the "solid" remains invariant with respect to the transformation that occurs in going between Fig. 1a and Fig. 1b. For this reason, in the presence of small perturbations associated with forces that result from outside interactions, a potentially huge degeneracy is present.

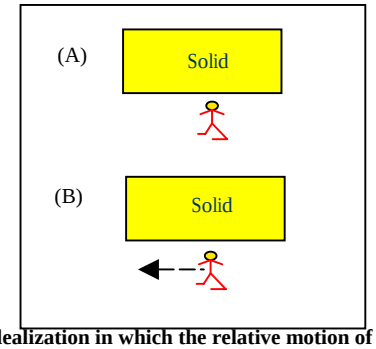

Fig. 1: Schematic Diagram of Idealization in which the relative motion of a solid and an observer is stationary (A) or in motion (B). As alluded to in the text, if the solid is required to be in its ground state, the "motion", schematically is required to involve the observer, alone.

Because the lowest energy system has smallest overlap with outside perturbations, system energy is required to be reduced through a reduction in translation symmetry. Enhanced coherence is a direct consequence of this possibility. In particular, for example, at temperature T=0, all particles in the solid have a common velocity V, and at the "boundary" of the solid, a change in the velocity of one particle through a minor perturbation couples to all of the particles. In this way a seemingly short-range, well-screened variation in the local electromagnetic interaction at one location, in fact, can have a large effect at distant locations. Thus, potential forms of coherence can result because rates of reaction are reduced when coherence from symmetry is allowed. A useful rule-of-thumb is: these forms of coherence are strongly correlated with the behavior of the charge; when charge does not build up, coherence can occur; when it does, coherence usually disappears.

In fact, preferentially, charge does build up at the boundaries of the solid, and this causes a reduction in symmetry. How this occurs involves a balance between the electrostatic forces and available momenta (p), and the velocities of individual particles (in Eq. 1) in the presence of collisions. In particular, collisions are allowed to occur through abrupt (quasi-discontinuous) changes in p. In principle, locally, these can be accompanied by compensating changes in A. However, when the total charge within a particular region vanishes and no further charge is found outside the region, near the Ground State, T=0, limit, changes in velocity must become proportional to changes in momentum.

In principle, through considerations, based on symmetry, it is possible to identify the boundaries of a solid in the T=0 limit, rigorously, and approximately at finite T, based on rules[8] (associated with the lowest forms of excitation) that asymptotically are required as $T \rightarrow 0$. This can be further quantified through a generalization of a well-known band theory, technique, Multiple-Scattering[7,8]. This theory applies at all values of T. But it requires detailed calculation[7] at elevated values of T. Slightly above T=0, a simplified form of this theory applies[8]. In this limit, the theory implies useful information about how and when charge can become localized that can be inferred by allowing the total momentum P (of the "bulk region") to acquire an imaginary component in regions where net charge can be appreciable (which is true in surface regions). Then, no net charge accumulates in bulk regions, where it is allowable for many charges to move in a rigid or quasi-rigid manner (as in Fig. 1b, and Eq. 2); while in surface regions, P can acquire an imaginary component, which leads to a dissipation of energy and momentum.

3 Potential Role of Broken Gauge Symmetry at Boundaries in the Iwamura et al Experiments

The situation in which the momenta p associated with the electrons that accompany the diffusing D in the Iwamura et al experiments[4] acquire imaginary components in directions perpendicular to the Pd surface is intriguing. Two possible results that apply in this limit are: 1. A form of highly anisotropic trapping might occur, in which each electron associated with each D could effectively become dissociated from its nuclear center (d) in directions parallel to the surface of the Pd (and Cs) but remain localized in the vicinity of its nuclear center in directions normal to the surface; and 2. Through potential degeneracy associated with gauge symmetry, that coherent coupling might occur between this (an-isotropic) configuration and perturbations that are directed normal to the surface.

4 Suggestions for New Experiments Based on the Potential Role of SBGS in the Iwamura et al Transmutation Work

A poorly-understood effect associated with the experiments[4] by IW involves the role of the CaO layers, within the interior of the Pd. In fact, if the kind of surface-localization effect, alluded to in the last section, is important, the CaO layers could become very important, as a potentially stabilizing force, in the electro-deposition of Cs. In particular, although these layers are positioned at a distance that is macroscopically finite from the Cs, in the context of conventional quantum mechanics, as it applies in atoms and molecules, in solids, the associated distance has marginal consequence. This is because except within the immediate vicinity of each surface or interface, the substrate effectively "behaves" as if it is neutral. For this reason, electrostatic effects can propagate over macroscopic distances in an effectively un-attenuated manner.

The role of the Cs-5p core electrons in the associated interaction may be important. In particular, although intuitively one might think that these electrons would not appreciably alter the bonding characteristics (much less the potential for nuclear reaction) associated with the (outer) Cs 6s electrons, in fact, they are known to be actively involved in the lowering of work function that occurs when Cs is deposited on the surface of many transition metals[5,6]. Thus, it is also not at all unreasonable to expect that the excitation of core electrons in the XPS process that is used to identify the concentrations of Cs (and/or Pr) atoms might be playing a potential role in triggering a longer-range, coherent form of coupling between the localized D's that are found in the immediate vicinity of the Pd surface, near the Cs, and the electronic/ionic charge associated with the CaO layers that are located far from the Cs-surface, within the Pd-bulk-like region. Two intriguing ideas for testing these hypotheses exist: 1. It is possible that by using a different set of core levels (and excitation energies) to monitor the presence of Cs, the reaction might disappear or be enhanced; 2. By varying the amount of CaO and/or the CaO separation from the Cs-Pd

surface, it might also be possible to alter the reaction process. Studies that alter both, or either, could be useful for identifying whether or not (or to what degree) longer-range effects are playing a role in the experiments.

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