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Theoretical Framework for Anomalous Heat and ^{4}He in Transition Metal Systems

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Introduction

Cold Fusion has been plagued with misconceptions about what is and is not possible, based on the "Laws" of Quantum Mechanics. An important reason for this is the seemingly impossibly large difference in length-scale between nuclear- and atomic- processes. In conventional fusion, these scales remain "so far apart" that they "effectively" don't "talk" to each other, usually. However, electromagnetic interactions (EMI's) have infinite range. For this reason, it is possible that EMI's "can" "explain" how this "apparent" problem can be eliminated.

A somewhat surprising feature of EMI's also is they can do this in the "seemingly" impossible situation in which "each of the particles" that is involved "effectively" has vanishingly small momentum. A key point in understanding how this can become possible is associated with how "momentum" and "length-scale" are related to each other. Although at high energy, the relationship between these quantities can be "viewed" as being localized, this is because when the associated Debroglie wavelengths ($\lambda_{Debroglie}$'s) of "individual particles" do not have appreciable overlap, the momentum p of an individual "particle" can be treated in terms of a classical picture, in which p=mv, where m is the mass of the particle, and v is its velocity.

As p-> 0, this picture breaks down because "uncertainties" in p and position (x) become intertwined with the electromagnetic field. For this reason, boundary effects and symmetry, through (implicit and explicit) EMI's lead to forms of coherence that explain well-known effects (Mossbauer effect, super-conductivity, Bragg-scattering, heat and electrical conductivity in solids) in which momentum can be shared by "many" "particles" "instantaneously." Because EMI's are also responsible for non-separable forms of coupling between electromagnetic and nuclear processes (in which the coordinates associated with these forms of forces depend on each other) in one form of reaction (D+D->^{4}He), it is theoretically possible that the two forms of interaction can become coupled. For this reason, it is also plausible that this form of interaction can become dominant in situations in which non-local, coherent effects that occur as p->0 (or when related limits, associated with large values of $\lambda_{Debroglie}$) become dominant.

An important point is that when the $\lambda_{Debroglie}$'s of many particles become sufficiently large (or are constrained by symmetry to particular values through the usual rules of Quantum Mechanics), coherent coupling between charged particles and an electromagnetic field can occur even in the limit in which the combined momentum of the particles becomes vanishingly small. The associated effect can explain how momenta can be transferred from an isolated location to many locations, all at once, without high energy being transmitted to any individual location. We explore the associated implications of this on Cold Fusion-related phenomena.

"Inside and Outside the Box" and the "Organizing Principles" of "Conventional Fusion"

Logical thought requires "rules." In physics, the logical "rules" follow from Newton's laws of motion, Maxwell's Equations, Quantum Mechanics, and Relativity. Because these "rules" provide a framework, often they can be self-limiting. For example, sometimes physicists misinterpret the "rules," simply because they are conditioned to look at them in a particular way. They become "used to" a particular "worldview." The "worldview" can be thought of as a kind of "box" that defines a "comfort zone." Often, the "box" is tied to the way we have learned a particular subject. Different people view the "box" in different ways. Kuhn[1] refers to it, abstractly, as it relates to science, as a "paradigm." Others have not been as open-minded[2].

Fig. 1 shows a pictorial representation of "conventional" fusion reactions super-posed on an idealized representation of the "box", associated with what is commonly viewed as "conventional" (labeled "inside the box") and "unconventional" (labeled "outside the box") science. In this schematic, all reactions originate from a configuration in which two deuterons (shown as proton-neutron pairs) overlap with each other in a manner that forms a configuration (shown in the center of the plot) that resembles an excited state of a ^{4}He nucleus. The two, dominant reactions (D+D->^{3}He+n, and D+D->^{3}H+p) that occur in free space are essentially "blind" to the presence of the electromagnetic interaction (EMI). For this reason, it is possible to treat these reactions within a framework in which the dependence of the reaction on electromagnetic interactions is independent of its dependence on the nuclear (strong force) interaction. This means that in these reactions, the associated wave functions describing the initial and final states do not couple the nuclear and electromagnetic interactions. As a result, the general reaction rate expression (which is described below) effectively "precludes" the "strong force" from "talking" to the "electromagnetic force," by construction. The figure schematically illustrates this point through the labels ("ignore E. M."),

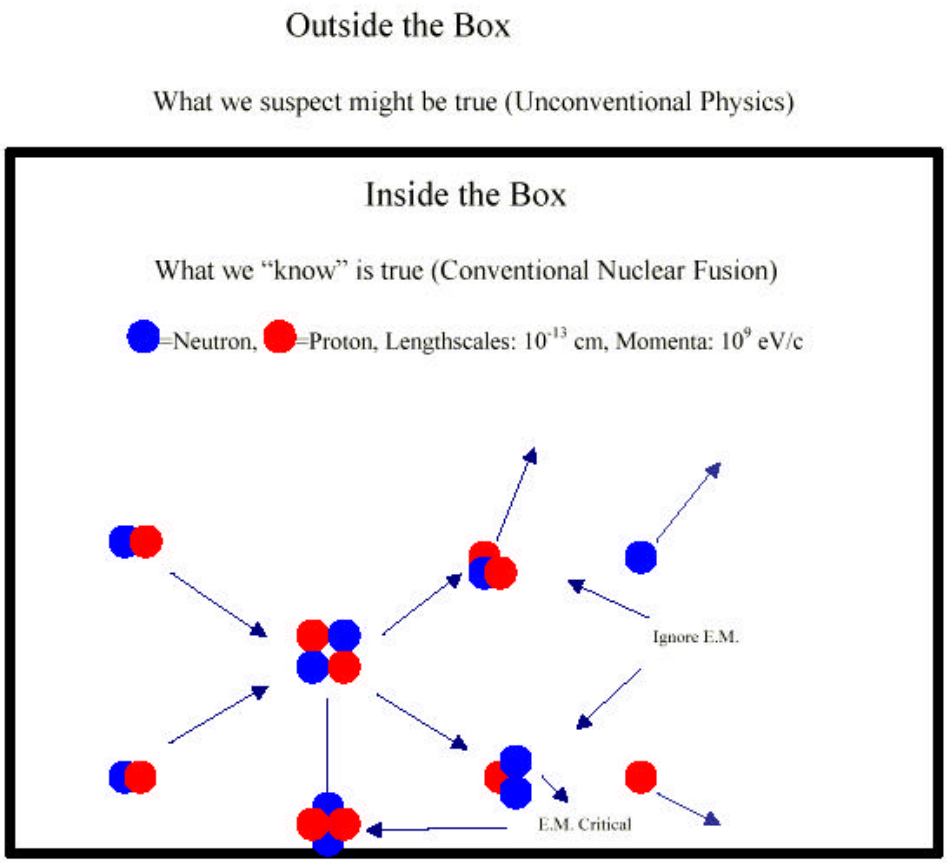

Fig. 1: Pictorial representation of conventional fusion reactions. Darkened and lightened circles, respectively represent neutrons and protons.

next to the arrows that are shown in the right portion of the figure. Also shown is the remaining fusion reaction (D+D->^{4}He). This reaction occurs rarely in conventional fusion. For this reason, in the figure it is shown as occurring at the "boundary" of the "box". A second reason we have drawn it at the boundary is that it violates a "paradigm" that many nuclear physicists believe to be valid: in conventional fusion, the strong and electromagnetic interactions remain uncoupled. For this reason, it is widely believed that the final (D+D->^{4}He) reaction should rarely occur and the two remaining

reactions should occur with roughly the same probability. However, the D+D->^{4}He does occur, and the reason that it is not frequently observed is well-understood: it violates energy-momentum conservation unless a high energy momentum gamma ray is emitted, and the associated EMI involves a complicated (quadrupolar) coupling between nucleon spins (that occurs as a second order electromagnetic process). Two important points are: 1. although this final reaction occurs infrequently relative to the others, when it occurs, the "nuclear" and "electromagnetic" interactions do "talk to each other", and 2. it occurs rarely because the associated processes involve overlap between two "particles" at a single location.

Motivational Physics for Getting Outside the Box

Part of the confusion with the "box" associated with conventional nuclear physics involves the definition of momentum p: for a single charged particle, p does not equal mass (m) times velocity (v); the "rules" of the "box" are: for a particle possessing charge q, mv=p-q/cA, where A (the vector potential) is associated with the electromagnetic interaction, and c is the speed of light. Although this rule is based on classical physics, how and where it applies "seems" to have been a source of confusion. The "rule" follows from the "box" defined by classical physics. (Miss-assumptions about this rule not only "appear to have led to confusion about Cold Fusion" but to more serious problems.)

An example of the importance of this distinction occurs in the p->0 limit, when "many" particles "share" a common density r_o. When this occurs, mv, which is proportional to the current J (provided r_o is uniformly constant[3]), becomes proportional to A. But A, which is defined by the static wave equation ($-\nabla^2 A \equiv \frac{4pJ}{c}$), then obeys a Helmholtz equation[3] ($-\nabla^2 A \equiv \frac{-4pq^2 r_o A}{mc^2}$) that results in A asymptotically vanishing beyond a critical coherence length, where J approaches a constant value. This occurs even in the absence of an applied electromagnetic field (EMF). The resulting picture explains the phenomenon of super-conductivity. It also explains how as p->0, super-conductivity not only is present, but because the current vanishes at some boundary, surrounding the region where superconductivity occurs, the effects of boundaries may result in the expulsion of magnetic flux when p=0 (the Meissner effect) or flux quantization[3], when p does not vanish but takes on values that are consistent with the associated rules (defined by "the box") associated with the requirements of quantum mechanics[3].

The basis of both phenomena is that p does not equal "mv"; in situations where the DeBroglie wavelengths of "particles" become sufficiently large, "particles" become "wavelike." In this kind of situation, the average value of the gradient of the phase of the associated collection of waves (which is described by the many-body wave function) defines the momentum. The important point is that the "phase of the many-body wave function," as opposed to a quantity related either directly to the current or to "mass x velocity" defines how the momentum behaves. When p->0, this quantity can be affected in ways that are non-local in character. This may occur because non-local changes in A can significantly alter the value of the phase. Because a priori it is not possible to predict if a solid is at rest or in motion, for example, its center-of-mass wave function can be altered by an arbitrary complex number. This introduces the possibility of an arbitrary gauge transformation in the definition of the A that applies inside and outside a solid. Because in the p->0 limit, it becomes possible to determine if the solid is in motion or at rest, the associated arbitrariness in "gauge" is removed. Not only does this mean that the associated "gauge symmetry" becomes broken, but physical effects (for example, the expulsion of magnetic flux, or spontaneous lattice recoil [as in the Mossbauer effect]) can occur. The resulting coherence can be viewed in different ways, within the framework (the "box") associated with a particular discipline.

In similar ways, effects of periodic order and other symmetries can become important in situations in which the wave-like character associated with large DeBroglie wavelengths becomes important. The important point is that because momentum is associated with wave-like behavior, it can change suddenly, in unexpected ways, on arbitrarily short time-scales. These changes can result in "instantaneous" changes in which large amounts of momentum coherently are shifted to many particles, and vice-versa. How or if this occurs is dictated by the dynamics of the many-body system.

More Precise Physics: Multiple Scattering

The exact problem is formidable. It involves solving the reaction rate problem for the (many-body) potential V that interacts with <u>all</u> charged particles. To understand how reaction rates in nuclear (as well as other) processes can be affected either through coherence that results as p->0 or (in a less restrictive sense) when symmetries constrain how p may vary during particular forms of interaction, it is not necessary to address all aspects of this problem. In particular, the associated coherence occurs as a result either of degeneracy or through the interactions between nearly degenerate states. The starting point of the analysis is general: we consider the problem of evaluating reaction rates, for a many-body system in which a perturbing potential V is present that asymptotically is assumed to have vanished in the distant past. Associated with the evaluation of reaction rate is the time evolution of the overlap $<E'^{-}|E^{+}>$ between an outwardly propagating many-body scattering state $|E^{+}>$ (defined by the assymptotic limit of the exact many-body state $|\Psi_E(t=time)>$: $|E^{+}> \equiv \lim_{t\to\infty}|\Psi_E(t)>$) with any of the possible initial, inwardly propagating states $|E'^{-}>$ ($\equiv \lim_{t\to-\infty}|\Psi_{E'}(t=time)>$). It follows from the asymptotic $(t\to\infty)$ limit of the well-known Lippmann-Schwinger equation that:

$$<E'^{-}(t)|E^{+}(t)> = <E'^{-}(0)|E^{-}(0)> + \frac{e^{\frac{-i(E-E'+ie\hbar)t}{\hbar}}}{E-E'+ie\hbar}<E'^{-}(0)|V|\Psi_E(0)> \qquad .(1)$$

Here, implicitly, $t\to\infty$, with the infinitesimal variable ε approaching zero, constrained by *1/e >t*.

In single-particle scattering theory, Eq. 1 is an integral representation of the Schroedinger equation. In many-body physics, it is equivalent to the Dyson equation, provided a "suitable" definition of V is employed. In fact, in practical applications involving many-body physics, V is never "known" exactly and is usually approximated using information provided by an approximate representation. Specifically, an important reason for using an approximate form for V is that usually neither V or $|\Psi_E(t)>$ is known explicitly. However, to address the more general problem of understanding how non-local interactions can evolve in many-body systems, it is not necessary to solve for either of these quantities. Instead, an alternative procedure, involving information associated with the underlying boundary conditions (and singular behavior of the wave function) may be employed. In this alternative formulation, "V" is replaced formally, using the kinetic energy operator $\hat{T}$ associated with the underlying many-body Schroedinger equations for $|\Psi_E(t)>$ and $|E^{-}(t)>$. This formal construction, which is a generalization of a standard, multiple-scattering technique[4,5], that has been applied in atomic, molecular, and solid state physics problems, in essence, relates the formal problem associated with scattering from a particular potential (as in Eq. 1) to a non-local momentum-balance problem. In this alternative problem, the matrix element $<E^{-}(t)|\ V\ |\Psi(t)>$ is transformed into a quantity involving $|\Psi_E(t)>$, $|E^{-}(t)>$ and the

derivatives of these quantities, evaluated at "boundaries" of the region, where V either becomes singular or vanishes.

Specifically, when $|\Psi_E(t)>$ satisfies the many-body Schroedinger equation associated with the many-body potential U, and energy E, it follows that

$$(H-\hat{T})|\Psi_E(t)>=(E-\hat{T})|\Psi_E(t)>''\equiv''U|\Psi_E>, \qquad (2)$$

where, in the coordinate representation, $\hat{T}=-\hbar^2\sum_i\frac{\nabla_i^2}{2m_i}$ (m_i is the mass of the ith particle (i=1,…,n)) is the many-body kinetic energy operator, and we have used the condition that $|\Psi_E(t)>$ is an eigenstate of *H*. Since a similar relationship holds when $<E'^{-}(t)|$ obeys a comparable Schroedinger equation associated with potential U', it follows that in a formal sense since $<E'^{-}(t)|V|\Psi_E(t)>\equiv<E'^{-}(t)|U-U'|\Psi_E(t)>$, that

$$<E'^{-}(t)|V|\Psi_E(t)>=(E-E')<E'^{-}(t)|\Psi_E(t)>+$$
$$+\int d^3r_1\int d^3r_2...\int d^3r_n\ \{\hat{T}\Psi^{-*}_{E'}(r_1,r_2...,r_n,t)\}\Psi_E(r_1,r_2...,r_n,t)-\Psi^{-*}_{E'}(r_1,r_2...,r_n,t)\{\hat{T}\Psi_E(r_1,r_2...,r_n,t)\} \qquad (3)$$

where $\Psi_E(r_1,r_2,...,r_n,t)\equiv<r_1,r_2,...,r_n|\Psi_E(t)>$, and $\Psi^{-}_{E'}(r_1,r_2,...,r_n,t)\equiv<r_1,r_2,...,r_n|E'^{-}(t)>$ are coordinate representations of $|\Psi_E(t)>$ and $|E'^{-}(t)>$.

Superficially, it might appear that the second term in Eq. 3 vanishes. In fact, this is not the case because of the implicit boundary conditions associated with Eqs. 1 and 2. In particular, because both the unperturbed and perturbed Hamiltonians are both Hermitean, E and E' are finite and real. But this means that at points where U and/or U' become singular, comparable singularities occur in the terms that involve $\hat{T}$ on the left-sides of Eqs. 2 and 3. As a consequence, surface terms (from discontinuities in one or more components of the gradients of one or both of the many-body wave functions) occur in the second term from regions that bound the locations where singularities in U and/or U' are present. Also, because $|\Psi_E(t)>$ and $|E'^{-}(t)>$ are not required to vanish (and may have appreciable overlap) in regions where U=U', it also follows that the second term on the right-side of Eq. 3 reduces to a sum of surface terms (through Greens theorem) at the boundaries of this region.

To understand the possible rates of reaction in Cold Fusion, we examine the situations associated with Eq. 1 in which the many-body states associated with $|E'^{-}>$ and $|E^{-}>$ are different. Because these states are different, the overlap matrix element $<E'^{-}(0)|E^{-}(0)>$ vanishes. This means that

$$|<E'^{-}(t)|E^{+}(t)>|^2=\frac{e^{2et}}{(E-E'+ie\hbar)(E-E'-ie\hbar)}|<E'^{-}(0)|V|\Psi_E(0)>|^2 \qquad (4)$$

from which it follows that

$$\frac{\partial|<E'^{-}(t)|E^{+}(t)>|^2}{\partial t}=\lim_{e\to 0}\frac{2e}{(E-E'+ie\hbar)(E-E'-ie\hbar)}|<E'^{-}(0)|V|\Psi_E(0)>|^2$$
$$=\frac{2p}{\hbar}d(E-E')|<E'^{-}(0)|V|\Psi_E(0)>|^2 \qquad .$$

$$\equiv \frac{2p}{\hbar} d(E-E') \left| \sum_i \iiint_{boundaries_i} d^{3n-1} r_i \quad \frac{\hbar^2}{2m_i} \hat{n}_i \bullet \{ \Psi^{-*}_{E'} \vec{\nabla}_i \Psi_E \quad - \vec{\nabla}_i \Psi^{-*}_{E'} \Psi_E \} \right|^2$$

$$\equiv \frac{2p}{\hbar} d(E-E') \left| < E' | \vec{\partial}_n | \Psi_E > \right|^2 \qquad .(5)$$

The total reaction rate R is constructed by summing the right side of Eq. 5 over all possible final (many-body) states *E*. The effects of coherence may enter when the initial state is formed from states that possess degeneracy. In particular, for example, this can occur when

$$E'_{\{k\}} \equiv \sum_k n_k e'(k) \qquad ,(6)$$

where *e'(k)* = energy of single-particle state possessing eigenvalue k; n_k = weighting factor that accounts for its degeneracy/occupation. In a many-body system, involving a macroscopic number of particles, $E'_{\{k\}}$ can be quite large, and, in general, when a sum is taken over all final states, many large and small terms can be involved on the right-side of Eq. 5. However, in situations where large degeneracy occurs in the initial state (and a small number of values of n_k can become large), a single term or a small number of terms can become dominant. An example of this kind of situation, for example, occurs when periodic order causes a large number of eigenvalues to be periodic functions with respect to the set of wave-vectors G (reciprocal lattice vectors) that define the Fourier transform of the underlying (periodic) potential because this form of symmetry can cause a significant number of states *e'(k)* to become degenerate: for example, *e'(k)* can = *e'(k+G)* for a large number N of values of G; in particular, N can ~ number of unit cells=N_{cell}. For illustrative purposes, suppose E'=N*e'(k)*. The resulting expression for the total reaction rate R is

$$R_{E' \to anything} = \frac{\partial P_{E' \to anything}}{\partial t} = \frac{2p}{\hbar} \sum_{k''} d(e'(k) - \frac{E(k'')}{N}) \frac{|<E'_{\{k\}}{}^{-}(0)|\vec{\partial}_n|\Psi_{E\{k''\}}(0)>|^2}{N} \qquad (7)$$

When discontinuities in $< E'^{-}_{\{k\}}(0) | \vec{\partial}_n | \Psi_{E\{k''\}}(0) >$ can be treated as if the associated states behave as band states, the right-side (R.S.) preserves periodic order. Then, the R.S. involves small, equal changes in momentum (or energy) from each unit cell. When the initial state concentration c_i of band state deuterons is sufficiently small, each matrix element scales as c_i; while the delta function, multiplied by 1/N (where N~Ncell) scales as the concentration c_f of final state, reactant products (e.g., band-state ^{4}He or ^{3}He), per unit cell. Thus, when $c_i{}^2 * c_f$ is sufficiently small in magnitude, the R.S. can become comparable to atomic timescales. (This occurs as a result of the non-local nature of the matrix element.) Then, when N~10^9 – 10^{10} unit cells (near temperature T=0), nuclear reactions can proceed at rates that can couple to atomic-scale processes, without high energy particles. For greater T, these kinds of reactions can occur at smaller values of N.

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