DEUTERON FLUXING AND THE ION BAND STATE THEORY

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Abstract

In Cold Fusion, confusion exists as a result of conflicting intuitive pictures, one based on local physics, the other on non-local physics. The local picture, based on particle-particle interaction, has played a dominant role. The non-local "less-intuitive" picture, based on the known behavior of solids, places greater emphasis on the behavior of matter distributions and their interaction with the associated environment. The resulting description is consistent with the known laws of physics and the behavior of hydrogen, deuterium (D^+) and tritons in transition metals. In the non-local picture, we examine consequences of fluxes of deuterons passing through the surfaces of transition metals as associated with the occupation of D^+ ion band states and possible nuclear energy release.

Introduction

Lattice Induced Nuclear Chemistry (LINC) explains[1] radiationless release of nuclear energy in a deuterided metal by a process in which deuterium converts to helium-4. This process occurs through self-interaction, based on a standard many-body formulation, provided coherent effects associated with periodic order (and the associated degeneracy) become important. Important features are embodied in the inherently non-local forms of interaction that may occur as a result of periodic order. In particular, coherence, broken gauge symmetry, as well as a number of non-local forms of interaction that are not usually considered in nuclear reactions, all may have consequence in periodically ordered systems. The explicit nature and significance of the associated interaction is considered in a separate paper that is included in this collection[2]. Because the non-local interaction can be related to the time evolution of the associated overlap between many-body wave functions[2], emphasis is placed on the wave functions and overlap characteristics. This provides an alternative framework that can be used to obtain insight into the associated physics.

In this paper, we use the non-local picture to obtain an intuitive understanding of phenomena associated with the breakdown of periodic order, especially the significance of non-equilibrium phenomena at locations where order breaks down and related effects. In the idealization of periodic order, the associated many-body system conforms to the periodicity of a host crystallite[1,3]. We emphasize that the assumed configuration of the deuterium matter is unlike that of chemical or interstitial hydrogen in normal metal hydrides.

Figure 1 illustrates some of the forms which matter can assume in response to embedding environments. The distributions are portrayed by their charge and mass distributions in space. Figs. 1a and 1b illustrate independent particle configurations.

a) b) c) d)

Fig.1 Mass and charge density distributions of various forms of matter

Fig. 1a shows the mass density of the nucleus of an atom in free space. The nucleus is roughly spherically shaped with a radius of the order of fermis, appearing as a point on the scale of the Bohr atom. The bottom sketch of Fig. 1b shows the same nucleus when bound inside a metal. In the lowest vibration state the nucleus assumes a Gaussian distribution inside a parabolic potential well. The distribution is called the zero-point motion distribution. The top sketch of Fig. 1b shows the charge and mass density distribution of the electron bound in a hydrogen atom. The distribution is called the ground state electron orbital. Figs. 1c and 1d illustrate composite particle entities, in which independent particles have joined together to form a new single entity. Fig. 1c illustrates a Bose-Einstein condensate made up of sodium atoms in a magnetic trap. The top sketch of Fig. 1d illustrates a portion of a Bose-Einstein condensate made up of sodium atoms in an optical trap. The optical trap is created by interfering laser beams that create a sequence of potential wells within which the Bose-Einstein entity resides. The Bose-Einstein condensate is partitioned so that only a fraction of the mass and charge of each sodium atom resides in any one potential well created by the interfering laser beams. The bottom of Fig. 1d shows the charge and mass distribution of a hydrogen ion on the surface of Ni 111. It is a partitioned composite entity, which is described by a Bloch function. The ion band state attributes radiation-less deuteron fusion to the self-interaction of a partitioned composite particle entity described by a many-body deuteron wave function.

Observation suggests fluxing deuterons

The ion band state theory predicted the radiationless fusion of deuteron pairings within a many body-wave function so as to form helium-4. Observations of helium-4 in the electrolysis off-gasses in electrolytic deuterium-palladium experiments have demonstrated the production of helium-4 sourced at a rate of ~24 MeV per helium atom produced. Although these observations are in agreement with the theory, many experimenters say that heat production is a non-equilibrium process. McKubre states. "You need to maintain a flux of deuterons through the interface. The phenomenon that we are studying is not an equilibrium phenomenon. It is a phenomenon that is stimulated by departure from the steady state." In his critique of the ion band state theory Bob Bush says, "You have to have a deuteron wind." Arata and Zhang attribute the success of their DS-cathode experiments to a rapidly diffusing form of deuterium called "spill-over deuterium". Heat-producing catalytic experiments using gas-loaded Pd-on-carbon catalyst are carried out in containers that do not maintain a constant temperature over the catalyst bed, which is conducive of a circulation of the deuterium through the bed. These experiments cause us to examine the role of deuteron fluxing in the observed heat production process.

A quantized matter field plus correlation

The physics of composite particle systems is modeled using second quantization theory in which a composite entity is described as a quantized matter field. In joining the composite entity, the separateness of the entering particles is lost. The quantized matter field is in turn described in terms of occupations of quantum states described by single particle wave functions. The occupations of the single particle states are called quasiparticles. The quasiparticles have the same charge and mass as that of the particles that joined into the composite entity. When the matter field is embedded in a metal crystal, the single particle states are solutions of the Schroedinger wave equation in which a charged particle is subject to a periodic potential provided by a host crystal lattice. The resulting wave functions are Bloch functions. When the many-body composite entity is composed of N_D deuterons in a crystallite containing N_{cell} unit cells of metal crystal, the lattice potential is modified by the distributed charge of the N_D added electrons provided by the N_D deuterium atoms and by the (N_D-1) positive charges associated by the (N_D-1) deuterons other than the test deuteron under consideration. The energy minimized Bloch function solution to this potential is called the mean field approximation wave function. The ion band state theory is concerned with small concentrations $D^+{}_{Bloch}$/Pd of Bloch function deuterons. At small concentrations using wave functions based on the bare lattice potential gives an adequate description of the system. It is important to note that this quantized matter field modeling is distinct from the modeling of a set independent particles subject to exchange. When all the quasiparticles are in the same state, all the single particle wave functions have the same distribution in physical space. This contrasts with and is inconsistent with the side-by-side distributions describing distinguishable, independent deuterons in a D_2 molecule.

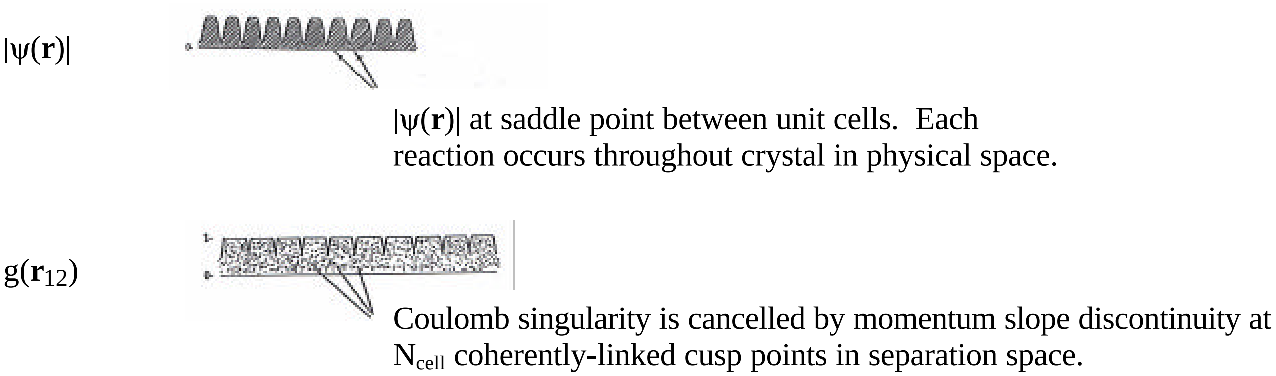
Despite its success, the quantized matter field description of a many-body system composed of Bloch function ions in a lattice is an incomplete picture of a charged-particle many-body system. It does not contain the instantaneous point self-interaction between the multiple quasiparticles. The description does not include the point-particle interaction between quasiparticle pairs. To correct this deficiency point-particle interactions are added to the quantum field picture by including particle-particle correlation factors in the many-body wave function. For quasiparticle pairings inside metals the correlation factor modulates the strength of a 2-body wave equation in response to the point-particle self-interaction attraction or repulsion potential. The controlling self-interaction potential is the Coulomb repulsion between paired particles e^2/r_{12}. The correlation factor reduces the amplitude of the 2-particle wave function when particle separation r_{12} is small. "Where particle$_1$ is, particle$_2$ mostly isn't." The d-d correlation factor also includes the nuclear attraction between paired deuterons if the deuteron pairing has zero nuclear spin. There is no separation of the electrostatic and nuclear potentials. The attractive potential comes into play at small separation provided the correlation factor does not reduce the 2-particle wave function to zero amplitude at $|\mathbf{r}_{12}| = r_{nuc}$, where r_{nuc} is the range of the nuclear force. However, this condition never occurs as long as periodic symmetry iunbroken. When periodic symmetry is broken, energy minimization selects the side-by-side D_2 molecule configuration.

The paired quasiparticle wave function

The 2-particle wave function describing pairings of quasiparticles is a 6-dimensional function. Pairings of quasiparticles can be written in terms of a 2-body wave function of the form

$$\Psi = \psi(\mathbf{r})\, g(\mathbf{r}_{12}) \,,$$

where $\mathbf{r}$ is the position vector in physical space and $\mathbf{r}_{12}$ is a separation vector in internal space. Here, $\psi(\mathbf{r})$ is a Bloch function in physical space and $g(\mathbf{r}_{12})$ is a Bloch function in separation space. In other words, $|\psi(\mathbf{r}+\mathbf{R}_j)|\,| = |\psi(\mathbf{r})|$ and $|g(\mathbf{r}_{12}+\mathbf{R}_{12})|\,| = ||g(\mathbf{r}_{12})|$, where $\mathbf{R}_j$ and $\mathbf{R}_{12}$ are independent Bravais lattice vectors. Figure 2 illustrates a possible form of $\psi(\mathbf{r})$ and $g(\mathbf{r}_{12})$. $\psi(\mathbf{r})$ has a maximum in each of N_{cell} unit cells of a crystallite in physical space, and has reduced amplitude at saddle points separating adjoining unit cells. $g(\mathbf{r}_{12})$ has a cusp-shaped minimum in each of N_{cell} unit cells of internal space in response to an $e^2/(N_{cell}^2\, r_{12})$ singularity in each of it N_{cell} coherence domain.Wave function Ψ transforms seamlessly into the 2-particle wave function describing a pair of independent non-interacting particles in the limit of large N_{cell} or of zero Coulombic potential self-interaction. The wave function is coherent over the N_{cell} volumes of physical and internal space. This means that calculation of physical quantities requires summing the contributions of both sets over N_{cell} unit cells.



$|\psi(\mathbf{r})|$ at saddle point between unit cells. Each reaction occurs throughout crystal in physical space.

Coulomb singularity is cancelled by momentum slope discontinuity at N_{cell} coherently-linked cusp points in separation space.

Fig. 2 Sketch of 2-quasiparticle wave function $\Psi = \psi(\mathbf{r})\, g(\mathbf{r}_{12})$ of Bloch function deuterons

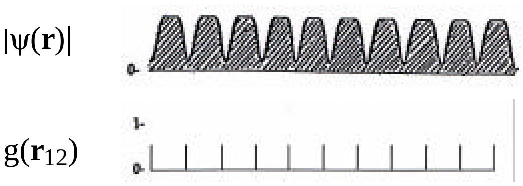


Fig. 3 The 2-quasiparticle wave function of Bloch function deuterons after coalescence

When a nuclear coalescence "reaction" occurs, a pairing of deuteron quasiparticles is replaced with a helium-4 nucleus in a reversible transition that preserves 2-particle Bloch symmetry. The periodic symmetry is preserved until irreversibility occurs by a dissipative process. The 2-deuteron wave function Ψ of Fig. 2 transitions reversibly into the coalesced form shown in Fig. 3. The cusps of function $g(\mathbf{r}_{12})$ become replaced with a repeated near-delta function configuration in which the deuterons are confined to a nuclear volume such that $|\mathbf{r}_{12}| < r_{nuc}$. The coalescence occurs at the set of N_{cell} cusp points in $g(\mathbf{r}_{12})$. The cusp points are points at which internal momentum is discontinuous, allowing momentum to be transferred out of the coherent many-body entity. Coalescence causes only a small change in the charge density distribution in physical space. The spatial distribution $\psi(\mathbf{r})$ is slightly altered by a change in zero point motion caused by a change in the quantum of mass and charge, and is accompanied by a steepening of the charge gradient at the ordered domain's boundary in physical space. The change in charge density couples the nuclear configuration to the lattice, enabling momentum transfer to the embedding environment by electron and/or phonon scattering.

Intuitive Picture for Role of fluxing deuterons

A non-zero value of Ψ at $\mathbf{r}_{12} = 0$ permits an approximate calculation of reaction rate using time dependent perturbation theory, assuming that coupling to a dissipative medium converts each coalescence into an irreversible fusion reaction. Deuteron fluxing does not directly enter into this idealized, periodically-ordered picture. So what is the role of deuteron fluxing? In the real world, deuteron fluxing plays a role as a result of broken periodic order. In particular, as we have discussed elsewhere[2,3], in the presence of boundaries, coherent lattice recoil may result in non-local transfer of momentum, playing a dominant role in the associated channels for reaction.

An intuitive picture of a potentially key role played by fluxing deuterons is that of creating and maintaining a non-fluxing population of ion band state deuterons inside a set of small ordered domains inside a metal matrix. The domains may be area-like or volume-like. It is conjectured that in the deuterium-palladium system at high D/Pd ratio there can exist 2 forms of fluxing deuterons. The first form is a normal population of interstitial deuterons that diffuse down their concentration gradient by tunneling transitions into adjacent empty octahedral sites. But it is conjectured that there is a second population of wavelike deuterons that are described by Bloch functions with charge density distributions concentrated outside the charge density maxima of the normal interstitials, possibly having significant charge density within the tetrahedral site volumes. These deuterons have high tunneling rates between unit cells. We associated the spillover deuterium described by Arata and Zhang with this second population. This second population could be an important diffusing component in palladium at high D/Pd loading, where there is a scarcity of the empty sites needed for normal diffusion. It is speculated that this population could be formed on electrolysis cell cathodes at an overvoltaged interface between the electrolyte and the cathode surface.

This intuitive picture is based on transposing results from modeling by Jaksch et al. of atoms in an optical lattice.[4] The Jaksch modeling describes an array of potential wells created by interference between 2 standing waves from laser beams of slightly different wavelength. The superposition of the 2 standing waves creates an amplitude-modulated sequence of strong E-field volumes that serve as energy traps for cold polarizable atoms. Atoms collected in the section of the array where the traps have their greatest depth is modeled in terms of a periodic distribution of matter constrained to have an equal mass content in a sequence of adjoining traps. The partitioned matter field is studied as a function of potential well depth and tunneling rates across the barriers between adjacent traps. The modelers find that 2 types of composite matter can co-exist in such an array. Type 1 is called a superfluid and is characterized by a fractional occupation of each individual trap. Type 2 is called a Mott insulator, which is characterized by a common whole number occupation of each trap. When the trap depth is relatively shallow and the tunneling rate high, the superfluid matter type dominates. When the traps are deep and separated by higher barriers, type 2 matter type dominates. When both types of matter are present, the different types of matter are spread out in different portions of the traps, i.e., where the Mott insulator charge density is relatively high, the superfluid matter density is relatively low, and vice versa. Transferring this picture to the metal lattice, we associate low density ion band state matter with the superfluid, and the normal interstitial deuterons at high D/Pd loading with the Mott insulator type of matter with single atom occupancy in each trap.

If this intuitive picture of high mobility Bloch function component of fluxing deuterons exists at high D/Pd ratio, we can analyze the deuterons using a boson version of the physics of electron current flow in metals. Treating such deuterons as quasiparticles of a quantized matter field, their time varying distribution in physical and momentum space is characterized by a distribution function G(**r**,**k**,t) where **r** is a location in physical space and **k** is a momentum index identifying a wavelike state. The many-body medium is subject to scattering where there are discontinuities in the hosting lattice environment. Scatterings at inhomogeneities are responsible for the resistivity of metals to electron current flow at low temperature. The interface between a highly ordered crystallite and a less ordered metal matrix constitutes an inhomogeneity for fluxing deuterons. The inhomogeneity subjects the many-body system to scattering events, changing G(**r**,**k**,t). Scattering events can remove deuterons from the fluxing population while adding deuterons to a non-fluxing distribution N(**k**) within the ordered domain. With bosons there can be a build-up of the **k**=0 zero-momentum population. This build up adds to a resident non-fluxing ion band state population within the crystallite. (A non-fluxing population can also exist when there is a balanced population of +**k** and -**k** state occupations.) A self-interacting long lasting N(0) population provides a possible explanation for "heat-after-death".

In addition to its role in populating D^+ ion band states, a fluxing Bloch function population of deuterons may be able to directly interact nuclearly with a resident population of non-fluxing deuterons. The 2 populations share the same set of k momentum states when in the same volume, but with different occupation distributions. Occupants need not be in the same k-state to interact. Also, a fluxing Bloch function population of deuterons exists as a many-body system without the presence of a resident population and can nuclearly self-interact just like a resident population. However, the density of the fluxing Bloch function population is likely to be much lower than the density of the non-fluxing population. Experiments are needed to determine the direct heating role of a fluxing Bloch function population.

References

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