

## Anomalous Nuclear Reactions and Atomic Processes in Transition-Metal Hydrides and Deuterides

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### Abstract

Formation of neutron energy bands in PdH (D) crystal originated in excited states of neutrons in Pd lattice nuclei (nuclei on the lattice points) is formulated using data in nuclear physics and in solid state physics. Neutron bands below the zero energy (neutron valence bands) are formed by the super-nuclear interaction between nuclei (the interaction between excited neutrons in lattice nuclei) mediated by occluded hydrogen isotopes. Neutrons in the bands show local coherence in boundary regions and form neutron drops (clusters of neutrons with a few protons and electrons) there in the sample. The neutron valence bands and neutron drops explain characteristics of nuclear reactions in solids including the so-called cold fusion phenomenon (CFP) different from those of nuclear reactions in the isolated nucleus studied extensively in nuclear physics. Possible applications of the anomalous nuclear reactions in solids are discussed.

### 1. Introduction

The nuclear structure of isolated nuclei in the energy region up to several hundred MeV has been thoroughly investigated in about ninety years to accomplish its fundamental understanding in the energy region up to several hundred MeV<sup>1,2)</sup> after the discovery of the atomic nucleus in 1911. The global features of the energy levels of nucleons and their distribution seem to be fairly well described by the Fermi-gas model,<sup>1)</sup> despite a fact "various experiments utilizing high-energy incident particles have attempted to explore this distribution but the results, so far, have been mainly confined to light nuclei, and a quantitative analysis is plagued with difficulties in the description of the reaction mechanism." (Ref.(1) Sec. 2-1c) It is true even now especially for excited levels with energies very close to the zero level; which corresponds to the neutron level with a binding energy of zero in the nucleus  ${}^A_ZX$ , or to the state where a neutron and the separated nucleus  ${}^{A-1}_ZX$  remain still. (We use this energy standard in this paper unless otherwise stated.) Therefore, it is interesting

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to have some phenomena which are directly related with the highest excited levels of nucleons in medium and heavy nuclei.

In the Fermi-gas model, excited levels of nucleons and the total level density in a nucleus are fairly extensively investigated<sup>1)</sup> for an isolated nucleus in a free state. When a nucleus is in stationary influence of interactions with other particles, on the other hand, nucleon states in the nucleus may be influenced largely by this interaction; especially, the positive charge density of external particles makes excited levels of a proton higher than that of a neutron. This may appear if the nuclei (lattice nuclei) are at lattice points interacting with hydrogen isotopes at interstices (occluded hydrogen isotopes) in transition-metal hydrides and deuterides.

In addition to the change of energy levels of nucleons in the nucleus, the effects of the external particles can cause coupling of a nucleon in a nucleus with another in a different nucleus, both in interaction with the same external proton or deuteron. In the case of transition-metal hydrides and deuterides (e.g. PdH (D) that we mainly treat in this paper), neutrons in excited levels of adjacent lattice nuclei can be coupled each other through interactions with the same occluded proton (deuteron).<sup>3)</sup> This interaction may be called "the super-nuclear interaction" in analogy with the super-exchange interaction between the electron spins of metal ions mediated by spins of oxygen ions in transition-metal oxides, e.g. MnO.

The super-nuclear interaction between neutrons in adjacent lattice nuclei results in the energy band structure of neutrons described by Bloch waves, which are depicted by the tight-binding approximation well known in solid state physics.<sup>4)</sup> An opposite limit of the approach to figure out the neutron band structure is the free-neutron approximation as presented in a previous paper.<sup>5)</sup>

Interesting features of neutron band structures appear in boundary regions of a crystal when there are reflecting walls; local coherence of neutron Bloch waves, and therefore, a high density of neutrons appear there.<sup>6)</sup> High density neutrons in the boundary region<sup>7)</sup> or in neutron star matters<sup>8)</sup> induce formation of neutron drops (or clusters of neutrons with a few protons and electrons) in a thin neutron background.

These features of high density neutrons in boundary regions might be participating in the so-called cold fusion phenomenon (CFP), i.e. more precisely expressed "nuclear reactions and accompanying events occurring in solids with high densities of hydrogen isotopes in ambient radiation."<sup>6,9)</sup> A model (the trapped neutron catalyzed fusion (TNCF) model) proposed by the present author was successful to give unified consistent explanation of CFP not only in deuterides but also in hydrides<sup>10,11)</sup> and premises assumed in the model have been investigated microscopically using the neutron band concepts.<sup>3)</sup>

In this paper, a quantitative verification of treatments given in previous papers<sup>3,10,11)</sup> is given on the knowledge of nuclear structures established in nuclear physics. We use the Fermi-gas model for nuclei throughout this work.

## **2. Excited States of Neutrons and its Density of States in Medium and Heavy Nuclei**

It is a common knowledge in nuclear physics that average properties of the excitation spectrum of nucleons in a nucleus are given by the Fermi-gas model as a

result of dominance of the particle degrees of freedom over the number of collective modes.<sup>1)</sup>

In the Fermi-gas model, nucleons in a lattice nucleus at  $\mathbf{a}_i$  is treated as independent particles and their quantum states  $\psi_{\{n\}}(\mathbf{r}-\mathbf{a}_i)$  are specified by quantum numbers  $\{n\} \equiv (n, \ell, m)$  omitting spin parts for simplicity;<sup>12)</sup>

$$\psi_{\{n\}}(\vec{r}-\vec{a}_i) \equiv \psi_{nlm}(\vec{r}-\vec{a}_i). \quad (1)$$

The wave function of a neutron in a nucleus  ${}^A_Z\text{X}$ , however, extends far away from the nucleus when the energy  $E$  of the state is less than but close to zero and then the wave function outside the nucleus is approximated by

$$\psi_{\eta,\ell,m}(\vec{r}-\vec{a}_i) = c_i e^{-\eta|\vec{r}-\vec{a}_i|} Y_{\ell,m}(\theta_i, \phi_i), \quad (2)$$

where  $\eta \equiv \eta(|E|)$  is a damping factor of the radial wave function depending on the energy but assumed for simplicity to be independent of quantum numbers, and  $(\theta_i, \phi_i)$  are angles measured from the lattice point  $\mathbf{a}_i$ . In the following treatment, we use the wave function (1) until we need the wave function (2).

The result of the calculation of the total level density for the Fermi gas is given as;<sup>1)</sup>

$$\rho(N, Z, \varepsilon) = \frac{6^{1/4}}{12} \frac{g_0}{(g_0\varepsilon)^{5/4}} \exp\left\{2\left(\frac{\pi^2}{6}g_0\varepsilon\right)^{1/2}\right\} \quad (N \approx Z), \quad (3)$$

where  $\varepsilon$  is the excitation energy measured in relation with the ground state and  $g_0$  is the one-particle level density at the Fermi energy  $\varepsilon_F$  representing the sum of the proton and neutron level densities:

$$g_0 \equiv g(\varepsilon_F) = \frac{3}{2} \frac{A}{\varepsilon_F}, \quad (4)$$

for a case  $Z = N = A/2$ .

The energy range where the above formula is applicable is determined by a relation

$$\frac{\varepsilon_F}{A} \ll \varepsilon \ll \varepsilon_F A^{1/3}, \quad (5)$$

where  $\varepsilon_F \simeq 37$  MeV for heavy nuclei. This relation gives an energy range of applicability  $0.4 \sim 170$  MeV for nuclei with mass numbers  $A \sim 100$ .

High density of nuclear levels at high excitation energies, amounts of the order  $10^6$  times higher than that corresponding to single-particle motion, has been revealed by densely spaced, sharp resonance in the slow neutron capture reactions in a nucleus with  $A \sim 100$ .<sup>1)</sup> The figure  $10^6$  will be increased further by several orders when the energy of the slow neutron capture reactions goes down to  $\sim 1$  eV. In the following discussion, we will take this factor as  $10^9$  at its maximum suggested by experimental data for Ag in the range of 2 to 8 MeV<sup>13)</sup> considering later application to Pd isotopes in the energy range up to 10 MeV.

This means, in terms of the Fermi-gas model, the compound nucleus corresponds to very extensive configuration-mixing in the stationary states and resonance. As a result, configuration-mixing will remove the selection rules associated with single

configurations. This fact about an isolated nucleus is very important in the investigation of phenomena related with these excited states in coupled lattice nuclei treated in the next section.

### 3. Effective Potential for the Super-nuclear Interaction between Neutrons in Adjacent Lattice Nuclei of Transition-Metal Hydrides and Deuterides

In the transition-metal hydrides (deuterides), the crystal structure is dependent on the concentration of hydrogen isotopes which can be introduced continuously into the crystal until a definite limit and kept stable there (occluded); the critical composition is PdH (D) in Pd, NiH (D) in Ni, TiH<sub>2</sub> (D<sub>2</sub>) in Ti, and so on.<sup>14,15)</sup>

The samples of transition-metal hydrides (deuterides), which we are interested in, are those with near critical compositions and we confine our investigation to crystals of stoichiometric compounds PdH (D) for our object in the following treatment. In this compound, hydrogen isotopes occluded in the crystal occupy octahedral interstices having six Pd atoms as nearest neighbors on the crystallographic axes half way of the lattice constant. The lattice constant  $a$  of the compound PdH <sub>$x$</sub>  depends on the composition  $x$  and is a little larger than that of Pd crystal 3.89 Å. In the following treatment, however, we ignore the dependence of the lattice constant on the composition and use the value for Pd crystal as for the compounds PdH <sub>$x$</sub> .

The nuclei of the transition-metal element on the lattice points (lattice nuclei) have six hydrogen isotope nuclei (protons or deuterons) as nearest neighbors at interstices half lattice constant 1.95 Å apart. The proton (deuteron) at an interstice is described as a three-dimensional harmonic oscillator in its ground and lower excited states and is sometimes described by proton (deuteron) Bloch waves in its excited states.<sup>16)</sup> The wave function of a proton (deuteron) in a state specified by quantum numbers  $\{p\} \equiv (n_p, \ell, m)$  at an interstice  $\mathbf{b}_j$ ,  $\varphi_{\{p\}}(\mathbf{R} - \mathbf{b}_j)$ , has finite probability density at nearby lattice nuclei especially when it is in excited states.<sup>3)</sup> If we ignore mutual interaction of protons (deuterons) in different interstices, the total proton (deuteron) wave function may be expressed as a product of wave functions on the interstices as follows with  $\{p_\alpha\} = (p_1, p_2, \dots, p_Z)$ ;

$$\Phi_{\{p_\alpha\}}(\vec{R}_1, \vec{R}_2, \dots, \vec{R}_Z) = \prod_j \varphi_{\{p_j\}}(\vec{R}_j - \vec{b}_j). \quad (6)$$

The overlapping of the proton (deuteron) wave function  $\varphi_{\{p\}}(\mathbf{R}_j - \mathbf{b}_j)$  on the interstice  $\mathbf{b}_j$  with a nucleon (neutron) wave function  $\psi_{\{n\}}(\mathbf{r} - \mathbf{a}_i)$  of an adjacent lattice nucleus at  $\mathbf{a}_i$  results in the proton (deuteron)-neutron interaction through the nuclear force.

The nuclear force is expressed by the gradient of a potential  $V(\mathbf{r} - \mathbf{R}_j)$  whose form is taken as one of following potentials;

$$\begin{aligned} V_{sw}(\vec{r} - \vec{R}) &= -V_0^{(s)}, \quad (|\vec{r} - \vec{R}| < b) \\ &= 0, \quad (|\vec{r} - \vec{R}| > b) \quad (\text{Square well}) \end{aligned} \quad (7)$$

$$V_G(\vec{r} - \vec{R}) = -V_0^{(G)} e^{-|\vec{r} - \vec{R}|^2 / r_0^2}, \quad (\text{Gaussian well}) \quad (8)$$

$$V_Y(\vec{r} - \vec{R}) = -\kappa \frac{e^{-|\vec{r}-\vec{R}|/r_0}}{|\vec{r} - \vec{R}|}, \quad (\text{Yukawa well}) \quad (9)$$

where  $V_0^{(s)} \sim 3.5$  MeV,  $b \sim 2.2 \times 10^{-13}$  cm,  $V_0^{(G)} \sim 3.5$  MeV,  $r_0 \sim 1.4 \times 10^{-13}$  cm and  $\kappa/r_0 \sim 3.5$  MeV.<sup>17)</sup> The choice of a potential from them does not make a large difference to the result for low energy phenomena<sup>12,17)</sup> we consider in this paper and we use  $V_{sw}(\vec{r} - \vec{R})$  hereafter.

This interaction brings two nucleons (neutrons) in lattice nuclei on different lattice points in coupling with each other which we named the super-nuclear interaction as explained in Introduction. In the following investigation, we concentrate on neutrons in lattice nuclei than protons which are in lower levels in the ground state due to the general rule  $Z < N$  and need more energy for excitation to levels around zero.

To investigate properties of the super-nuclear interaction between neutrons in different nuclei, we use the tight-binding approximation for excited neutrons in lattice nuclei. In a periodic potential of lattice nuclei, a neutron in an excited level of a lattice nucleus is described quantum mechanically as a linear combination of states centered at each lattice nucleus with the same probability and its state is expressed by a Bloch function;

$$\psi_{\vec{k}}(\vec{r}) = \sum_i e^{i(\vec{k}\vec{a}_i)} \psi_{\{n\}}(\vec{r} - \vec{a}_i). \quad (10)$$

Therefore, the total wave function of a system composed of a neutron Bloch wave and  $Z$  protons at interstices is expressed as follows (neglecting spin parts of wave functions, for simplicity);

$$\Psi_{\vec{k},\{p_\alpha\}}(\vec{r}; \vec{R}_1, \vec{R}_2, \dots, \vec{R}_Z) = \psi_{\vec{k}}(\vec{r}) \Phi_{\{p_\alpha\}}(\vec{R}_1, \vec{R}_2, \dots, \vec{R}_Z), \quad (11)$$

The description of neutrons by the Bloch functions becomes a good approximation when the band width finally obtained is wide enough to make the neutrons move freely in the crystal not disturbed by perturbations causing aperiodicity in the periodic potential of the lattice nuclei. The origin of the perturbation will be lattice imperfections (caused by deviation from PdH (D) composition), thermal oscillation of the lattice nuclei, impurity atoms, and so on.

The neutrons in excited states of lattice nuclei and occluded protons (deuterons) at interstices could be treated independently because an exchange of the neutron and the proton results in fairly high-energy states and does not occur with high probability. The total energy  $E_{\vec{k},\{p_\alpha\}}$  of the system with a neutron in a band state  $k$  and protons in states  $\{p_\alpha\}$  in this approximation is expressed as follows in the second-order perturbation calculation taking the square-well potential (7) for the nuclear potential:

$$E_{\vec{k},\{p_\alpha\}} = E_{\{n,p_\alpha\}} + \sum_{k',i',j} \exp(-i(\vec{k}\vec{a}_i - \vec{k}'\vec{a}_{i'})) v_{np}(ii'j), \quad (12)$$

$$v_{np}(ii'j) = \sum_{n',p'} \times \frac{\langle np; ij | V | n'p'; ij \rangle \langle n'p'; i'j | V | np; i'j \rangle}{E_{\{n',p'\}} - E_{\{n,p\}}}, \quad (13)$$

$$E_{\{n,p_\alpha\}} = E_{\{n\}}^{(p)} + \sum_j \varepsilon_{p_j}, \quad (14)$$

$$V(\vec{r}) = V_s(\vec{r}), \quad (15)$$

$$\begin{aligned} \langle np; ij | V | n'p'; ij \rangle &= \int \int d\vec{r} d\vec{R}_j \vec{\psi}_{\{n\}}^*(\vec{r} - \vec{a}_i) \varphi_p^*(\vec{R}_j - \vec{b}_j) \\ &\quad \times V(\vec{r} - \vec{R}_j) \psi_{\{n'\}}(\vec{r} - \vec{a}_i) \varphi_{p'}(\vec{R}_j - \vec{b}_j), \end{aligned} \quad (16)$$

where summations over  $i$  and  $i'$  are only over the nearest neighbor lattice points  $\mathbf{a}_i$  and  $\mathbf{a}_{i'}$  of the interstice  $\mathbf{b}_j$ , summations over  $\{n', p'\}$  exclude the term where the denominator becomes zero,  $E_{\{n\}}^{(p)}$  is an energy of a neutron in an excited state  $\psi_{\{n\}}(\mathbf{r} - \mathbf{a}_i)$  in a lattice nucleus at  $\mathbf{a}_i$  when protons are in states  $\{p_\alpha\}$ , and  $\varepsilon_{p_j}$  is an energy of a proton in a state  $\varphi_{p_j}(\mathbf{R}_j - \mathbf{b}_j)$  at an interstice  $\mathbf{b}_j$ . The neutron energy  $E_{\{n\}}^{(p)}$  can be approximated by the energy of a neutron in a lattice nucleus interacting with protons in a state  $\bar{p}$ , an average of  $p_i$ 's because  $|E_n| \gg |\varepsilon_p|$ . We ignore, however,  $p$ -dependence of  $E_{\{n\}}^{(p)}$  hereafter in this work ( $E_{\{n\}}^{(p)} = E_{\{n\}}$ ).

For quasi-continuous levels of excited states in a lattice nucleus, we have to calculate such a following integral excluding a point where the denominator becomes zero to obtain the effective potential energy  $v_{np}(ii'j)$  (13);

$$\begin{aligned} &\sum_{\{n'\}, \{p'\} \neq \{n\}, \{p\}} \frac{\langle np; ij | V | n'p'; ij \rangle \langle n'p'; i'j | V | np; i'j \rangle}{E_{\{n', p'\}} - E_{\{n, p\}}} = \sum_{\{p'\} \neq \{p\}} \\ &\times P \int_{-\infty}^{\infty} dE \rho_n(E) \frac{\langle np; ij | V | n'p'; ij \rangle \langle n'p'; i'j | V | np; i'j \rangle}{E + \varepsilon_{p'p}}, \end{aligned} \quad (17)$$

where  $\rho_n(E)$  is the level density of excited states for a neutron,  $\varepsilon_{p'p} = \varepsilon_{p'} - \varepsilon_p$ , and  $E = E_{\{n'\}} - E_{\{n\}}$ . Further, the summation over  $\{p'\}$  reduces to  $(n_p+1)(n_p+2)$ , the degeneracy of the energy  $\varepsilon_{n_p}$ , times summation over  $n_p$ .

To specify the neutron wave functions  $\psi_{\{n\}}(\mathbf{r} - \mathbf{a}_i)$  to calculate matrix elements in the above equation, we utilize knowledge obtained in the shell model calculation. We use the Fermi-gas model with the nuclear harmonic oscillator potential. Then, the wave functions and energy eigenvalues specified by quantum numbers  $(n, \ell, m)$  are written down as follows;<sup>12)</sup>

$$\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell, m}(\theta, \phi), \quad (|m| \leq \ell) \quad (18)$$

$$E_{\{n\}} \equiv E_{n\ell m} = \left(n + \frac{3}{2}\right) \hbar \omega_n + \Delta \varepsilon_{\ell m}, \quad (19)$$

where  $\Delta \varepsilon_{\ell m}$  expresses the  $l \cdot s$  and other coupling energies taken symbolically into consideration to distinguish energies of the states with the same  $n$  and different  $\ell, m$ ,  $\omega_n$  is the circular frequency of the nuclear harmonic oscillator and  $Y_{\ell, m}(\theta, \phi)$  are the spherical harmonics.

The spherical harmonics  $Y_{\ell, m}(\theta, \phi)$  are given as follows;

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}, \quad (20)$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad Y_{0,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}, \quad (21)$$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1), \quad Y_{2,\pm 1} = \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\phi},$$

$$Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi}, \quad (22)$$

$$Y_{3,0} = \sqrt{\frac{7}{16\pi}} (5 \cos^3 \theta - 3 \cos \theta), \quad Y_{3,\pm 1} = \mp \sqrt{\frac{7}{48\pi}} (15 \cos^2 \theta - 3) \sin \theta e^{\pm i\phi},$$

$$Y_{3,\pm 2} = \sqrt{\frac{105}{32\pi}} \cos \theta \sin^2 \theta e^{\pm 2i\phi}, \quad Y_{3,\pm 3} = \mp \sqrt{\frac{105}{112\pi}} \sin^3 \theta e^{\pm 3i\phi}. \quad (23)$$

In nuclei of palladium isotopes, there are excited neutron states  $2f_{7/2}$  and  $3p_{3/2}$  near zero as shown by shell model calculation with a Woods-Saxon potential.<sup>1)</sup> Concrete calculation of the effective potential energy  $v_{np}(i'l'j)$  (17) will be performed for these levels with wave functions;

$$\psi_{2f_{7/2}}(r, \theta, \phi) = R_{53}(z)Y_{3,m}(\theta, \phi), \quad (|m| \leq 3) \quad (24)$$

$$\psi_{3p_{3/2}}(r, \theta, \phi) = R_{51}(z)Y_{1,m}(\theta, \phi), \quad (|m| \leq 1) \quad (25)$$

$$R_{53}(z) = c_n \left(\frac{32}{210}\right)^{1/2} z^{3/2} \left(1 - \frac{2}{9}z\right) \exp^{-z/2}, \quad (26)$$

$$R_{51}(z) = c_n \left(\frac{35}{12}\right)^{1/2} z^{1/2} \left(1 - \frac{4}{5}z + \frac{4}{35}z^2\right) \exp^{-z/2}, \quad (27)$$

$$c_n = 2\left(\frac{8\alpha_n^3}{\pi}\right)^{1/4}, \quad z = 2\alpha_n r^2, \quad \alpha_n = \frac{m_n \omega_n}{2\hbar},$$

where  $m_n$  is the mass of the neutron and  $\omega_n = 41/A^{1/3}$  MeV.<sup>12)</sup>

For the interstitial proton (deuteron) wave functions  $\varphi_{\{p\}}(\mathbf{R}-\mathbf{b}_j)$ , on the other hand, we use harmonic oscillator wave functions in a three-dimensional spherical potential centered at an interstice determined by using diffusion data.<sup>16)</sup>

$$\varphi_{\{p\}}(\vec{R}) = \varphi_{n_p \ell m}(R, \Theta, \Phi) = \xi_{n_p \ell}(R)Y_{\ell, m}(\Theta, \Phi), \quad (28)$$

$$\varepsilon_{n_p \ell m} = \left(n_p + \frac{3}{2}\right)\hbar\omega_p, \quad (29)$$

or by Hermite polynomials  $H_n(\xi)$ ;

$$\varphi_{\{p\}}(\vec{R} - \vec{b}_j) = u_{n_x}(x)u_{n_y}(y)u_{n_z}(z), \quad (30)$$

$$u_n(x) = N_n H_n(\alpha x) \exp(-(1/2)\alpha^2 x^2), \quad (31)$$

$$\alpha^4 = m_p K / \hbar^2, \quad N_n = \left(\frac{\alpha}{\pi^{1/2} 2^n n!}\right)^{1/2}. \quad (32)$$

where  $\mathbf{R} = (R, \Theta, \Phi)$ ,  $n_p$  is an integer,  $\ell \leq n_p$  and  $|m| \leq \ell$ ,  $\varepsilon_{n_p \ell m}$  is the proton energy of the state  $\varphi_{n_p \ell m}(\mathbf{R})$ ,  $\omega_p = (K/m_p)^{1/2}$  with the force constant  $K$  and the proton (deuteron) mass  $m_p$  and  $n_i$  ( $i = x, y$  or  $z$ ) are integers. The wave functions thus determined include already effects of screening by itinerant and bound in atoms electrons and also Coulomb repulsion by lattice nuclei.

The analysis based on the diffusion data<sup>16)</sup> showed that appropriate wave functions for a proton (deuteron) in the PdH (PdD) is that with  $n_p = 2$  (3) in the above expression and corresponding force constants  $K$  are given as

$$K_H = 1.44 \times 10^{19} \text{ eV/m}^2 \text{ (PdH)}, \quad K_D = 1.22 \times 10^{19} \text{ eV/m}^2 \text{ (PdD)}. \quad (33)$$

The relevant wave functions are written down as follows;<sup>1,12)</sup>

$$\varphi_{1d}(R, \Theta, \Phi) = \xi_{1d}(Z)Y_{2,0}(\Theta, \Phi), \quad (n_p = 2) \quad (34)$$

$$\varphi_{2s}(R, \Theta, \Phi) = \xi_{2s}(Z)Y_{0,0}(\Theta, \Phi), \quad (n_p = 2) \quad (35)$$

$$\varphi_{1f}(R, \Theta, \Phi) = \xi_{1f}(Z)Y_{3,0}(\Theta, \Phi), \quad (n_p = 3) \quad (36)$$

$$\varphi_{2p}(R, \Theta, \Phi) = \xi_{2p}(Z)Y_{1,0}(\Theta, \Phi), \quad (n_p = 3) \quad (37)$$

$$\xi_{1d}(Z) = c_p \left(\frac{4}{15}\right)^{1/2} Z \exp^{-Z/2}, \quad (38)$$

$$\xi_{2s}(Z) = c_p \left(\frac{3}{2}\right)^{1/2} \left(1 - \frac{2}{3}Z\right) \exp^{-Z/2}, \quad (39)$$

$$\xi_{1f}(Z) = c_p \left(\frac{8}{105}\right)^{1/2} Z^{3/2} \exp^{-Z/2}, \quad (40)$$

$$\xi_{2p}(Z) = c_p \left(\frac{5}{3}\right)^{1/2} \left(1 - \frac{2}{5}Z\right) \exp^{-Z/2}, \quad (41)$$

$$c_p = 2\left(\frac{8\alpha_p^3}{\pi}\right)^{1/4}, \quad Z = 2\alpha_p R^2, \quad \alpha_p = \frac{m_p \omega_p}{2\hbar}, \quad \omega_p = (K/m_p)^{1/2}.$$

It should be noticed that the determination of the proton (deuteron) wave function<sup>3)</sup> is tentative and should be revised when new data on the quantum mechanical states of hydrogen isotopes in transition-metal hydrides become possible to use.

A concrete expression of one of the matrix elements (16) for PdH is expressed using wave functions (24), (25), (34) and (35) as follows;

$$\begin{aligned} & \langle 2f_{7/2}1d; ij | V | 3p_{3/2}2s; ij \rangle \\ &= - \int \int d\vec{r} d\vec{R}_j R_{53}(z_i) Y_{3,0}(\theta_i, \phi_i) \xi_{1d}(Z_j) Y_{2,0}(\Theta_j, \Phi_j) \\ & \quad \times V_{sw}(\vec{r} - \vec{R}_j) R_{51}(z_i) Y_{1,0}(\theta_i, \phi_i) \xi_{2s}(Z_j) Y_{0,0}(\Theta_j, \Phi_j), \\ z_i &= 2\alpha_n |\vec{r} - \vec{a}_i|^2, \quad Z_j = 2\alpha_p |\vec{R}_j - \vec{b}_j|^2, \end{aligned} \quad (42)$$

where  $\mathbf{a}_i$  is a nearest neighbor lattice site of the interstice  $\mathbf{b}_j$ ,  $K$  in  $\alpha_p$  is  $K_H$  given in (33), and  $(\theta_i, \phi_i)$  and  $(\Theta_j, \Phi_j)$  are angles measured from origins at  $\mathbf{a}_i$  and  $\mathbf{b}_j$ , respectively.

Similar expression for PdD using deuteron wave function with  $n = 3$  is written as follows if the neutron-deuteron interaction potential is written as  $V_{sw}^{(nd)}(\mathbf{r} - \mathbf{R}_j)$ ;

$$\begin{aligned} & \langle 2f_{7/2}1f; ij | V | 3p_{3/2}2p; ij \rangle \\ &= - \int \int d\vec{r} d\vec{R}_j R_{53}(z_i) Y_{3,0}(\theta_i, \phi_i) \xi_{1f}(Z_j) Y_{3,0}(\Theta_j, \Phi_j) \\ & \quad \times V_{sw}^{(nd)}(\vec{r} - \vec{R}_j) R_{51}(z_i) Y_{1,0}(\theta_i, \phi_i) \xi_{2p}(Z_j) Y_{1,0}(\Theta_j, \Phi_j). \end{aligned} \quad (43)$$



In this equation, the force constant  $K$  in  $\alpha_p$  should be taken as  $K_D$  given in (33).

Because the triton is much more tightly bound than the deuteron, the potential  $V_{sw}^{(nd)}(\mathbf{r}-\mathbf{R})$  in (43) should be deeper than  $V_{sw}(\mathbf{r}-\mathbf{R})$  in (42). For a qualitative calculation of the matrix element (43), we may use a following form for the potential;

$$V_{sw}^{(nd)}(\vec{r}-\vec{R}) = \xi V_{sw}(\vec{r}-\vec{R}), \quad (44)$$

where  $\xi$  is a numerical factor of an order of the ratio of binding energies of triton (8.5 MeV) and deuteron (2.2 MeV) reduced to per a nucleon;  $\xi \sim (8.5 \div 3) / (2.2 \div 2) \sim 2.6$ .

To calculate matrix elements (42) and (43), we use a simplified form of the neutron wave functions (24) and (25) using the Dirac delta-function;<sup>18)</sup>

$$\psi_{n\ell m}(r, \theta, \phi) = \left(\frac{2\delta(r)}{r^2}\right)^{1/2} Y_{\ell m}(\theta, \phi). \quad (45)$$

Then the integrals over  $\mathbf{r}$  can be done readily and the result for (42) is written as

$$\langle 2f_{7/2}1d; ij | V | 3p_{3/2}2s; ij \rangle = -V_0^s \int d\vec{R}_j \xi_{1d}(Z_j) Y_{2,0}(\Theta_j, \Phi_j) \xi_{2s}(Z_j) Y_{0,0}(\Theta_j, \Phi_j), \quad (46)$$

in which the integral should be done in a region where  $|\mathbf{R}_j - \mathbf{a}_i|$  is less than  $b$ , the range of the square-well potential. Similar expression for the matrix elements for deuterium system is obtained for (43) with an extra factor  $\xi$  in front of the integral on the right-hand side.

The order of magnitude of the effective potential energy  $v_{np}(ii'j)$  for PdH, however, is roughly estimated as follows: the proton wave function  $\phi_p(\mathbf{R})$  is slowly varying in the range of the nuclear force, and the nuclear wave function  $\psi_{\{n\}}(\mathbf{r})$  is approximated by a delta-function as given in above Eq.(45). Then, an order of magnitude of the matrix elements  $\langle np; ij | V | n'p'; ij \rangle$  is given as

$$| \langle np; ij | V | n'p'; ij \rangle | \sim \int \psi_n^* \psi_n d\vec{r} \langle V \rangle \phi_p^* \phi_p \Omega \quad (47)$$

$$\begin{aligned} &\sim 1 \times \frac{4}{3} \pi r_0^3 \times |u_2(x_N)|^2 |u_0(0)|^2 |u_0(0)|^2 \\ &= 3.2 \times 10^{-14} \text{ eV}, \end{aligned} \quad (48)$$

where  $\Omega$  is the volume of the Pd nucleus,  $\langle V \rangle = |V_0^{(s)}| = 3.5 \text{ MeV}$  (Eq.(7)),  $\phi_p(\mathbf{R})$  is taken as  $u_2(x)u_0(y)u_0(z)$  and  $x_N = 1.95 \text{ \AA}$  is the position of the lattice nucleus measured from the interstice.

Putting this value (47) into Eq.(17), we can estimate the effective potential energy  $v_{np}(ii'j)$  as a function of the principal value of the integration appeared in that equation, assuming the insensitiveness of the matrix elements to the energy:

$$v_{np}(ii'j) \sim 1 \times 10^{-27} (\text{eV}^2) I, \quad (49)$$

$$I \equiv P \int \frac{\rho_n(E)}{E} dE.$$

We can, then, estimate the approximate value of the integral  $I$ , taking following values  $\rho_n(E) \sim 10^9 \text{ keV}^{-1}$ ,  $\delta\varepsilon \sim 10^{-9} \text{ keV}$ , and  $\Delta\varepsilon \sim 1 \text{ keV}$  on the assumption that single particle energy level difference is  $\sim 1 \text{ keV}$  and the level density increases to  $10^9$  times larger than that of single particle motion:

$$I \sim \frac{\rho_n(\varepsilon)}{\delta\varepsilon} \Delta\varepsilon = 10^{15} \text{ eV}^{-1}. \quad (50)$$

Thus, an order of magnitude of  $v_{np}(ii'j)$  in PdH becomes

$$v_{np}(ii'j) \sim 1 \times 10^{-12} (\text{eV}). \quad (51)$$

The value of  $v_{np}(ii'j)$  in PdD may be taken as one order of magnitude larger than this value if we consider the factor  $\xi=2.6$  ( $\xi^2 = 6.8$ ) and  $u_3(x_N)$  instead of  $u_2(x_N)$  in Eq.(47).

#### 4. Tight-Binding Neutron Bands in Transition-Metal Hydrides and Deuterides

The approximate effective potential energy  $v_{np}(ii'j)$  obtained above is used to calculate the band structure of the neutron energy in transition-metal hydrides (deuterides) originated in the excited states of neutrons in lattice nuclei mediated by occluded hydrogen isotopes.

To show crystal-structure dependence of the band width, we can use a simplification of the super-nuclear interaction between adjacent nuclei assuming that it depends only on the magnitude of vectors  $(\mathbf{a}_i - \mathbf{a}_{i'}) \equiv \mathbf{a}_i$  (taking  $\mathbf{a}_{i'} = 0$ ). We can, then, rewrite the neutron parts of expression (12) as follows;

$$E = E_n - \alpha - \gamma \sum_i e^{-i(\vec{k}\vec{a}_i)}, \quad (52)$$

$$-\alpha = v_{np}(ij), \quad (53)$$

$$-\gamma = v_{np}(ii'j). \quad (54)$$

Neglecting direction dependence of the effective potential, we have the energy spectrum of neutron Bloch waves in the face centered cubic (fcc) lattice from this equation ( $a$  is the side of the cube);

$$\begin{aligned} E &= E_n - \alpha - 2 \times 4\gamma (\cos \frac{1}{4}k_y a \cos \frac{1}{4}k_z a \\ &+ \cos \frac{1}{4}k_z a \cos \frac{1}{4}k_x a + \cos \frac{1}{4}k_x a \cos \frac{1}{4}k_y a) \\ &- 2\gamma (\cos k_x a + \cos k_y a + \cos k_z a), \quad (\text{fcc}) \end{aligned} \quad (55)$$

where summation over the index  $i$  is over neighbors combined each other by a proton (deuteron). The factor 2 in the third term on the right comes from the fact that nearest neighbor lattice nuclei are mediated by two protons at different interstices while next nearest ones are by only one. A characteristic of this energy band formation is the contributions from nearest  $(0, \pm a/2, \pm a/2)$  etc. and also from next nearest  $(\pm a, 0, 0)$  etc. neighbors to the  $\mathbf{k}$ -dependent terms.

The energy of a neutron consists, therefore, of a constant term  $E_n - \alpha$  and terms which depends on the wave vector  $\mathbf{k}$ . Thus, there exists a nuclear energy band in the crystal corresponding to an energy level of a neutron in the free nucleus when there are a high density of protons (deuterons) at interstices (ideally at each interstice). The effective potential energy  $v_{np}(ii'j)$  (13) gives a value of the integral  $\gamma$ , and hence the band width  $\Delta$  in metal hydrides. It should be noticed here that the band structure of neutron energy depends not only on the excited state of a neutron in lattice nuclei but also on the lattice structure; geometry of lattice sites and also interstices. The nuclear interaction of nuclei in metal hydrides (deuterides) is, therefore, influenced strongly by the symmetry and lattice constants of the crystal that can occlude hydrogen isotopes.

The neutron energy bands originating in excited states of lattice nuclei are located just below zero energy and contrasted to those originating from free neutron states above zero worked out in a previous paper.<sup>5)</sup> The former could be named *neutron valence band* and the latter *neutron conduction band* to distinguish them in the following discussion of the characteristic nuclear reactions in transition-metal hydrides and deuterides.

Using the value of  $v_{np}(ii'j)$  given in (51), we obtain a semi-quantitative estimation of the valence band width  $\Delta$  from Eq.(55):

$$\Delta = 24v_{np}(ii'j) \sim 10^{-8} \text{ (meV) (PdH)}. \quad (56)$$

Thus, it is concluded that the matrix elements (42) should be  $10^5$  times larger than the values estimated in (48) to substantially keep the neutron bands below zero which was determined to form in solids with a width  $\Delta \geq 25$  meV that is not destroyed by the thermal motion of ions at room temperature. This is realized only when the neutron wave function (1) extends out as the wave function (2) from a lattice nucleus to regions where a wave function of the occluded proton (30) has a larger value by a factor  $10^5$  than that at the lattice nuclei.

The main term of the proton wave function relevant to this behavior is the exponential factor  $e^{-\frac{1}{2}\alpha^2 x^2}$  in (31) and it gives this value  $10^5$  at  $x_0 = 1.43 \text{ \AA}$  from an interstice (or  $0.52 \text{ \AA}$  from a lattice point). If this behavior is coupled with an extension of the neutron wave function (2), then the neutron-proton interaction can contribute to formation of a neutron valence band with a width of  $\Delta \geq 25$  meV.

From a point of view of the isolated nucleus treated in conventional nuclear physics, this is an unconceivable situation. While, the extension of a neutron wave function (2) far away to  $0.52 \text{ \AA} = 5.2 \times 10^{-9} \text{ cm}$  over the nuclear range of  $r_0 = 10^{-13} \text{ cm}$ , i.e.  $10^4$  times longer than  $r_0$ , is not absurd in the situation we are considering here.

As was shown by numerical calculation in a previous paper,<sup>11)</sup> the energy of thermal neutrons interacting with lattice nuclei by the attractive nuclear force is pulled down below zero; the states of propagating waves then become quasi-localized states around lattice nuclei with a damping factor depending on the strength of the attractive interaction. The same situation is also realized from opposite direction as a limit of highest bound states as shown in Eq.(2). We consider here an s-type

wave function for the state, for simplicity:

$$\psi_\eta(\vec{r} - \vec{a}_i) = c_i e^{-i\eta|\vec{r} - \vec{a}_i|}. \quad (57)$$

To extend the neutron wave function to the range of  $\lambda = 5.2 \times 10^{-9}$  cm referred above, the decay constant of the state  $\eta(|E|) = 1/\lambda$  should be  $1.9 \times 10^8$  cm $^{-1}$  and this corresponds to an energy  $E$ :

$$|E| = \frac{\hbar^2}{2m_n} \eta(|E|)^2 = 7.4 \text{ (eV)} \quad (58)$$

below zero, where  $m_n = 1.67 \times 10^{-24}$  g is the neutron mass. In other words, the excited states of isolated lattice nuclei with energies down to 7 eV from zero can participate to *the neutron valence band*, or the neutron bands below zero, in transition-metal hydrides considered above.

If the state has less energy, i.e. far from zero, and the extension of the state is less than  $5.2 \times 10^{-9}$  cm, the band state fails to be substantially formed even in PdH and neutrons are essentially in single particle states in isolated lattice nuclei.

The width  $\Delta$  of the neutron band (55) is  $\sim 24\gamma = 24v_{np}(ii'j)$ . Putting the numerical values obtained in (42) for PdH and one for PdD by multiplying a factor of 10 to that of PdH as discussed on the end of Section 3, we obtain

$$\Delta = 10^{-8} \text{ (meV)} \quad (\text{PdH}), \quad (59)$$

$$\Delta = 10^{-7} \text{ (meV)} \quad (\text{PdD}). \quad (60)$$

Thus, these neutron states pulled down to just below zero from free states above zero by attractive interaction with lattice nuclei or excited states of lattice nuclei close to zero energy can be candidates of those states participating the neutron valence bands below zero in transition-metal hydrides considered above.

Matrix elements of similar interactions between a neutron in the ground state at its highest level (e.g.  $2d_{5/2}$  in  $^{106}\text{Pd}$ ) and an interstitial proton (deuteron) in the excited state are written down as follows;

$$\begin{aligned} & \langle 2d_{5/2}1d; ij | V | 1g_{7/2}2s; ij \rangle \\ &= - \int \int d\vec{r} d\vec{R}_j R_{42}(z_i) Y_{2,0}(\theta_i, \phi_i) \xi_{1d}(Z_j) Y_{2,0}(\Theta_j, \Phi_j) \\ & \quad \times V_0^{(G)} e^{-|\vec{r} - \vec{R}_j|^2/r_0^2} R_{44}(z_i) Y_{4,0}(\theta_i, \phi_i) \xi_{2s}(Z_j) Y_{0,0}(\Theta_j, \Phi_j). \end{aligned} \quad (61)$$

A numerical calculation of this matrix element gives a little smaller value than that of the above one (48). This is also easily confirmed as follows. The matrix element (16) with proton (deuteron) wave function of the ground state  $\varphi_{1s}(\mathbf{R}) = \xi_{1s}(Z) Y_{00}(\Theta, \Phi)$  is estimated using a nature of harmonic oscillator wave functions that the mean-square displacement in the n-th excited state is proportional to the energy of that state.<sup>19)</sup> Therefore, the matrix elements for PdH (the second excited state) and for PdD (the third) in these ground states become 1/5 of the value of (42) and 1/7 of the value of (43), respectively, which we have not estimated exactly.

The effective potential energy  $v_{np}(ii'j)$  (13) of the super-nuclear interaction corresponding to the matrix elements (61) is, however, extremely small compared with that corresponding to (42) or (43) due to the factors  $\rho_n(E)$  in (17) and the denominator  $(E_{n',p'} - E_{n,p})$  of terms in the summand of (13). The value of  $\rho_n(E)$  in (17) is  $10^6$  times larger than that we expect for the occupied highest levels (e.g. for  $2d_{5/2}$  in  $^{106}_{46}\text{Pd}$ ) of the ground state and accordingly the denominator of (13) is larger by the same factor. The result of these two causes gives  $10^{-12}$  smaller values for the effective potential  $v_{np}(ii'j)$  and therefore the band width  $\Delta$  even if the matrix element (61) has a value of the same order of magnitude with that of (42). Thus, the lattice nuclei in their ground state are best described as an ensemble of isolated independent nuclei as treated usually in solid state physics.

## 5. Cold Fusion Phenomenon in Transition-Metal Hydrides and Deuterides

The neutrons in a band show several characteristics when they are in a crystal with a finite extension limited by reflecting walls which are formed at boundaries of a crystal or at interfaces of two crystals having different nature.<sup>6)</sup>

First of all, neutrons with wave vectors around Brillouin zone boundaries have local coherence in a definite length (a coherence length) at the reflecting boundary. The local coherence produce an accumulation of high-density neutrons in the boundary region with a finite width, of an order of the coherence length, which is determined by the structure of the dispersion relation of the band neutron; the narrower the energy band, the larger the coherence length as far as the band is an effective concept to describe the neutrons. The effective minimum band-width  $\Delta_{min}$  may be given by thermal energy of the lattice  $kT$ ;  $\Delta_{min} \sim kT$ . The expected density of neutrons in the coherence region is estimated<sup>7)</sup> from experimental data in CFP as high as  $10^{30} \text{ cm}^{-3}$  to form clusters of neutrons with a few protons (neutron drops).<sup>7,8)</sup>

The new state of neutrons in solids discovered in this and previous works<sup>3,6,7)</sup> will show various novel phenomena induced by its interactions with lattice nuclei. One of these phenomena should be the so-called cold fusion phenomenon (CFP) observed mainly in transition-metals and proton conductors including a lot of hydrogen isotopes.

It has been a long controversy about reality of the CFP, i.e. nuclear reactions and accompanying events occurring in solids with high densities of hydrogen isotopes in ambient radiation,<sup>6,9)</sup> since the announcement of its discovery of some events belonging to CFP in samples of palladium deuteride.<sup>20)</sup> In these more than twelve years, it is shown that CFP occurs not only in the deuterium system, mainly transition-metal deuterides supposed at first as one of necessary conditions for CFP, but also in the hydrogen system mainly transition-metal hydrides with sufficient contents of hydrogen isotopes above lower limits of their content. The lower limit in PdD seems around  $\text{D/Pd} \sim 0.7$ .<sup>21)</sup>

The phenomenon is, further, characterized by following properties.<sup>6,9,10,21)</sup>

1) It occurs sporadically and with qualitative reproducibility. The former means that its occurrence is not predictable while the latter that the effects be distributed

in its yield from null to a maximum for the same macroscopic initial condition.

2) The events in CFP is classified into direct and indirect events in relation with presumed nuclear reactions. The former events directly show occurrence of nuclear reactions in the system and are composed of the energy spectra of gammas and neutrons from the samples and also spatial distributions of nuclear products in them. The latter events indirectly show occurrence of nuclear reactions and are composed of the huge excess heat, inexplicable by atomic and/or chemical processes, and large amount of helium-4 and tritium in addition to transmuted nuclei not specified its position of birth.

3) There are definite relations between products of these events. Let us denote the number of an event  $X$  as  $N_X$ , and define  $N_Q$ , number of the event producing the excess heat  $Q$  (measured in MeV) by

$$N_Q \equiv Q/5(\text{MeV}).$$

There are, then, following relations between  $N_X$ , experimentally observed amounts of  $X$  ( $^4\text{He}$ , tritium, transmuted nuclei) and  $N_Q$ ;

$$N_Q \sim N_X. \quad (62)$$

4) Nuclear reactions responsible to the CFP seem to occur in localized regions of a diameter of a few  $\mu\text{m}$  in the near-surface layer of thickness less than  $10 \mu\text{m}$  which is determined experimentally by distribution of transmuted nuclei and also by principal measurement of  $^4\text{He}$  outside the samples. The thickness of the near-surface layers are about few  $\mu\text{m}$  up to about  $10 \mu\text{m}$ .

5) Amount of gammas is very few compared with amounts of observed  $^4\text{He}$ , tritium, and transmuted nuclei, therefore, with that of the excess heat. This characteristic is called *gammaless nuclear reactions* in CFP.

It is necessary, then, to seek a key mechanism to explain CFP both in transition-metal hydrides and deuterides if we want to treat them in the same frame and not try to seek different mechanisms for each system.

There is a phenomenological model, named the TNCF model (trapped neutron catalyzed fusion model), which is fairly successful in explanation of various phases of CFP.<sup>9~11,21)</sup> The model is constructed on several premises based on experimental facts. One of fundamental premises is existence of quasi-stable neutrons in solids (trapped neutrons) with a density  $n_n$ , which is taken as a single adjustable parameter. In a few optimum cases where measured several events simultaneously, the single adjustable parameter  $n_n$ , fortunately, could be determined uniquely to explain them consistently as a whole.

The values of  $n_n$  determined by experimental data sets, more than sixty sets as a whole,<sup>11,21)</sup> are in a range  $10^8 \sim 10^{13} \text{ cm}^{-3}$ . This figures compared with number of lattice nuclei of the order of  $10^{23} \text{ cm}^{-3}$  (e.g.  $\sim 6.8 \times 10^{22} \text{ cm}^{-3}$  in Pd metal) give relative values of  $10^{-15} \sim 10^{-11}$  for trapped neutrons to lattice nuclei ratio; as a result, one neutron per  $10^{11} \sim 10^{15}$  lattice nuclei is necessary to explain CFP by the mechanism assumed in the TNCF model. Excitation of neutrons of this ratio

into the neutron valence bands from lattice nuclei could be realized by trigger reactions initiated by neutrons fed into the neutron conduction band from background neutrons as discussed in the explanation of TNCF model.<sup>9~11,21)</sup>

The phenomenological assumption of quasi-stable neutrons in solids, in turn, has suggested fundamental mechanisms causing CFP in samples with above mentioned characteristics, especially in transition-metal hydrides and deuterides. Investigation of behaviors of neutrons in solids given in previous<sup>3,5,7)</sup> and this papers revealed new features of neutron physics.

The calculation done in this paper has given rather quantitative verification of the basis of the TNCF model; it is shown that a neutron in an excited state of a lattice nucleus can be coupled with another in a corresponding state of another lattice nucleus by the super-nuclear interaction mediated by occluded protons (deuterons) and there appear band states of these neutrons. The neutron Bloch waves in these energy bands are responsible to CFP just the same way as these quasi-stable trapped neutrons assumed in phenomenological explanations of characteristics of CFP in previous papers.<sup>6,9~11)</sup>

## 6. Discussion

First of all, it should be kept in mind following facts about anomalous nuclear reactions in solids. The cold fusion phenomenon (CFP) is most frequently observed in transition-metal deuterides and hydrides, especially in TiD (H), NiH (D), and PdD (H). Furthermore, these transition-metal nuclei have a common characteristic; existence of excited neutron levels near zero in an isolated nucleus,  $1f_{5/2}$  in Ti,  $3s_{1/2}$  in Ni, and  $2f_{7/2}$  in Pd.<sup>1)</sup> Therefore, the investigations on PdH (D) given in the preceding sections are straightforwardly applicable to such materials as TiD (H), NiH (D), and others with necessary modifications to meet characteristics of each material.

When there are many neutrons in a neutron band formed by characteristics of transition-metal hydrides and deuterides, there appear interesting features of neutron's behavior at boundaries/surfaces that reflect neutrons back into the crystal; "local coherence" of neutron Bloch waves, and therefore, high densities of neutrons appear there<sup>6)</sup>. High-density neutrons in the boundary region<sup>7)</sup> or in neutron star matters<sup>8)</sup> induce formation of "neutron drops" (or clusters of many neutrons and a few protons) in a thin neutron background. These neutron drops in a thin neutron background interact with nuclei to produce new nuclear effects in the boundary/surface region.

In this paper, we have shown a new feature of neutron physics in transition-metal hydrides and deuterides using the physics of these compounds and of excited neutron states in nuclei. Based on the new knowledge, we can give a qualitative explanation of these riddles 1) to 5) in CFP written down in the previous section in addition to other nuclear reactions characteristic to solid state-nuclear physics completely different from physics of an isolated nucleus.

a) It is necessary to have such ordered structures of appropriate lattice nuclei and occluded hydrogen isotopes as PdH (D) or TiH<sub>2</sub> (D<sub>2</sub>) to realize neutron valence bands below zero. The transition-metal nuclei should have high-density excited

neutron levels around zero energy. It is necessary, also, to excite occluded interstitial protons (deuterons) to excited states, to the second (the third) one in PdH (PdD). The process of appropriate structure formation, even in local region, contains stochastic atomic processes and the optimum structure is established only with *qualitative reproducibility*.

b) To trigger CFP (i.e. to excite enough neutrons into the neutron valence band), it is necessary to have a few trapped neutrons in a neutron conduction band above zero,<sup>6,9,21)</sup> perhaps, fed from the background neutron. The trapped neutrons in the neutron conduction band form neutron drops in the boundary region and react with hydrogen isotopes to produce enough energy to excite neutrons in lattice nuclei to the neutron valence bands. This process occurs *sporadically* governed by a probability law.

c) Neutrons in the neutron valence bands form, also, neutron drops in the boundary/surface region where occur various reactions responsible to events in CFP. The *locality* of nuclear products of CFP is natural results of this mechanism to induce nuclear reactions between neutron drops and nuclei in the sample; lattice nuclei, occluded hydrogen isotopes and nuclei deposited on the sample.

d) The energy liberated in nuclear reactions occurring in the boundary region are shared by nuclides coupled each other through the super-nuclear interaction and can be dissipated through various channels not confined to those known in isolated nuclei. The gammaless nuclear reactions in CFP is surely the result of this characteristic of nuclear reactions in nuclei coupled each other.

e) As a result of the neutron drop-nucleus interaction, a nucleus in its excited state can decay rapidly giving excitation energy to other particles in solids through neutron drops. The nuclear transmutation by decay and the decay-time shortening are observed in CFP as noticed by us.<sup>21)</sup>

f) The neutron drop-nucleus interaction results in also an unbelievable fission reactions in CFP. The nuclear transmutation by fission analyzed by us<sup>21)</sup> and by Fisher<sup>22)</sup> is the proof of this reaction.

The difference of the baand width  $\Delta$  of PdH and PdD given in Eqs.(59) and (60) tells us the latter is advantageous to realize CFP if other conditions are the same. This result seems in accordenace with experience obtained in a decade of CF research.

Furthermore, it is possible to deduce some interesting features of protium and deuterium systems depending on spins of the proton and the deuteron which we have neglected in the treatment given above, for simplicity. The neutron has a spin  $\frac{1}{2}\hbar$  and a magnetic moment  $-1.91315 \mu_0$ , the proton  $\frac{1}{2}\hbar$  and  $2.79278 \mu_0$ , the deuteron  $1 \hbar$  and  $0.8574 \mu_0$  and the triton  $\frac{1}{2}\hbar$  and  $2.98 \mu_0$  with the nuclear magneton  $\mu_0 = e\hbar/m_Nc$ . Therefore, a system composed of a neutron in an excited state of a lattice nucleus and an interstitial deuteron (e.g. PdD) is in lower energy state if they have opposite spin, or the same direction of magnetic moments, which is realized by application of a strong magnetic field to the system. This effect of magnetic fields to make feasible occurrence of CFP will be observed in deuterium systems (e.g. PdD) but not in protium systems (e.g. PdH).

In conclusion, scientifically, the cold fusion phenomenon (CFP) gives a mean to



investigate excited neutron levels near zero in transition-metal nuclei and also neutron energy bands derived from them by the super-nuclear interaction mediated by hydrogen isotopes. Knowing physical processes of CFP in transition-metal hydrides and deuterides, we can proceed to next steps in physics; improvement of qualitative reproducibility, enhancement of frequency of sporadic occurrence of events in CFP.

In technology, the physics of transition-metal hydrides and deuterides gives wide possibility to see their characteristics in application. Some examples are the necessary protection of hazardous radiation from the reaction systems, the effective remediation of radioactive nuclides produced in atomic piles, the effective production of tritium accompanied with heat production, and so on.

Finally, we would like to notice a new point of view; it should be considered that various events in CFP are results of measurements using various probes to look into physics of a complex system composed of transition metals and hydrogen isotopes occluded in them in ambient radiations. If we do not confine our investigation in a narrow scheme presupposed by a biased viewpoint, new perspective can be developed on the basis suggested by experimental facts, even if they seem too complicated at first sight to be treated consistently.

The treatment of palladium hydrides and deuterides in this paper is, of course, qualitative because it is confined to PdH and PdD with simplifying assumptions on wave functions  $\psi_{\{n\}}(\mathbf{r}-\mathbf{a}_i)$  and  $\phi_{\{p\}}(\mathbf{R}-\mathbf{b}_j)$  to make calculation feasible and also there are many approximations in calculations of integrals. The result, however, semi-quantitatively shows a possible appearance of the super-nuclear interaction and the neutron valence bands in transition-metal hydrides. The nuclear reactions induced by neutron drops interacting with nuclei should be very different from nuclear reactions observed in isolated nuclei well known in nuclear physics and will show new features of solid state-nuclear physics not well explored until now. The results are applied straightforwardly to other transition-metal hydrides and deuterides and proton conductors.

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