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Low Energy Nuclear Reactions (LENR) and Heavy Fermion Catalysis for a Cold Fusion

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**Abstract.** We consider in the paper an idea of a heavy fermions catalysis for a cold fusion similar to a muon catalysis.

**Key words:** heavy fermions, cold fusion, catalysis, hydrogen storage, low energy nuclear reactions, chemically assisted nuclear reactions.

In the paper we give an idea of a heavy fermion (heavy electron) catalysis for a (super)cold fusion. The idea is based on two pillars: muon catalysis (Ref. [1]) and cold fusion in palladium-hydrogen systems (Ref. [2]). In this approach we want to use heavy fermions from strongly electron correlated materials (Ref. [3]) as muons in muon catalysis, in some materials used for a hydrogen storage (Ref. [4]). In that way we want to get a fusion reaction catalysed by a heavy fermion and a situation where a density of deuterium is very high as in a hydrogen storage. Thus we need a material with heavy fermions and with a high affinity to hydrogen.

It is interesting that the idea of heavy fermions and low energy nuclear reactions appears in Ref. [5].

In the paper we consider a kinetics of low energy nuclear reactions in a condensed phase. This involves many different domains of physics and chemistry, e.g. chemically assisted nuclear reactions. This approach can be even extended to biology in a living cell via biochemistry. On the molecular level there is no difference between biology, chemistry and physics. In some sense everything is physics. The catalysis caused by heavy fermions in a condensed phase connects many aspects of solid state physics, nuclear physics and chemistry. Some considerations connected to free energy (free enthalpy) production due using of irreversible chemical thermodynamics can also be inspiring for researchers not particularly involved in a subject covered by the paper. The paper is primarily of a theoretical nature. Moreover, we give some ideas of an experimental setup to check the theory. Summing up, the paper comments many domains of physics, chemistry and even biology from both theoretical and experimental points of view.

We call this idea supercold fusion for a possibility that such materials can have strongly correlated electrons (coming to heavy fermion systems) not only in an ambient temperature but even in low temperatures (of liquid helium or liquid nitrogen). (This is possible for some of those materials are superconductors.) The possibility of heavy fermion systems is very exciting for an effective mass of a quasiparticle (a quasifermion) can be so high as  $1000m_e$  (electron mass). In this way we consider a quasiparticle (a heavy fermion) as a source of a quasichemical bond.

The idea of quasiparticles is a very powerful tool in physics from Hawking radiation theory (Bogolyubov transformation approach) to condensed matter physics and nuclear physics or even biophysics. It is very well known that in solid state physics electrons and holes can form bounded states—excitons. Quite recently we meet also new bounded states—trions formed from two holes and an electron or two electrons and a hole (see

Ref. [6]). They are analogues of H<sup>-</sup> or H<sub>2</sub><sup>+</sup> states. Some of researchers communicate to discover in experiments condensation of exciton gas to a liquid or even Bose–Einstein condensation of this gas. Excitons and trions can be considered as quasiparticles as well.

Our idea is to use quasiparticles approach to form more exotic molecules—bounded systems of two deuterons and one heavy fermion in a hydrogen storage material in order to proceed a controlled nuclear fusion in ambient temperature (maybe in low temperatures).

According to an international discussion on a cold fusion in palladium no one was able to repeat results from first two points of Ref. [2]. However some anomalous excesses in a neutron production have been reported.

Quasiparticles concept is strongly connected to condensed matter physics, e.g. solid state physics. They are related to highly complicated behaviour in a solid state by an analogy of a very simple picture, e.g. molecules forming a perfect gas in a container. Quasiparticles are usually considered as fermions (sometimes as bosons, but in this case they are usually called collective excitations). One can find very simple physical concepts of quasiparticles in Ref. [7]. In a solid state even electrons (which are "real" particles) should be considered as quasiparticles. Quasiparticles can interact. Moreover, the general idea is such that they interact weakly. Quasiparticles can interact with ordinary "real" particles. A typical example is an interaction (a scattering) of quasiparticles in a superfluid (a liquid helium 2) with neutrons discovered by L. D. Landau. The second very well known example is a scattering of photons (real particles) and phonons (quasiparticles) as a description of Raman effect in solids. Our approach is to use interactions of quasiparticles in a sample of a solid state material with ordinary particles like deuterons, protons etc. Moreover, there is a different approach (see Ref. [8]) where real interactions are considered between deuterons induced by a lattice palladium (PdH) or Ti lattice TiH<sub>2</sub>. In this approach effective potentials between Pd and H

$$V_{\text{Pd-H}} = \frac{22.2}{r} \,\text{eV} \cdot \mathring{A} \exp\left(-\frac{r}{0.42\mathring{A}}\right) \tag{1}$$

and between Ti and H

$$V_{\text{Ti-H}} = \frac{31}{r} \,\text{eV} \cdot \text{Å} \left( \exp\left(-\frac{r}{0.51\text{Å}}\right) + \left(\frac{r}{1.095\text{Å}}\right)^{10.57} \right) \exp\left(-\frac{r}{0.23\text{Å}}\right) \tag{2}$$

have been derived.

Due to these potentials it is possible to derive effective potentials between H and H (D and D). These potentials consist of two parts: repulsive and attractive

$$V_{\text{H-H}}(r) = V_{\text{R}}(r) + V_{\text{A}}(r) \tag{3}$$

$$V_{\rm R}(r) = \frac{e^2}{\varepsilon r} \left( \exp\left(-\frac{r}{D_S}\right) + \left(\frac{r}{r_{\rm R}}\right)^p \exp\left(-\frac{r}{D_i}\right) \right) \tag{4}$$

$$V_{\rm A}(r) = -\frac{e^2}{\varepsilon r} \left(\frac{r}{r_{\rm A}}\right)^q \exp\left(-\frac{r}{D_{\rm A}}\right) \tag{5}$$

 $(\varepsilon, D_S, r_R, r_A, D_A, p, q)$  are parameters). This approach is known as a dense plasma approach for a cold fusion. In this approach a tunnel effect is considered in the potential (3) for two deuterons to get a cold fusion.

Our approach is different for we consider "quasichemical bonds" in a sample of a solid state matter caused by a "heavy fermion"—a quasiparticle. Due to this "quasichemical bond" a quasimolecule of two deuterons is formed and a tunnel effect is similar as in a muon catalysis. In some sense this description is dual to the effective potential between two deuterons for a heavy fermion—heavy electron exists due to lattice interactions with real electrons.

In Ref. [8] the few-particle processes are considered as a cause of a cold fusion in contradiction to binary processes which are rather typical for a hot fusion. Our approach is also a few-particle process. Moreover one of the particles is a quasiparticle. Quasiparticle is a collective effect in condensed matter physics. In this paper we consider also the few-particle processes but with two stages. The first is a quasiparticle formation process and the second an interaction of a quasiparticle with real particles. The similarity with muon catalysis is evident and an analogue with chemical bond is natural. In this way our fusion process is a cold fusion process also in the terminology of Ref. [8].

Let us consider a hydrogen in heavy fermions (heavy electron) systems. In this way we consider an ionized hydrogen molecule bound by a heavy fermion (electron). This is similar to the  $\mu^-$  hydrogen molecule. Let us denote a heavy fermion by  $F^-$  and let a mass of the particle be  $m_F$ . Let us suppose that we have to do with a heavy isotope of hydrogen D. In this way we have to do with three bodies interactions  $F^-, d^+, d^+$  or  $F^-, d^+, p^+$ , where  $d^+$  denotes a deuterium nucleus (deuteron) and  $p^+$  is a proton. We need a bounded system of  $(d^+d^+F^-)^+$  or  $(d^+p^+F^-)^+$  being an analogue of  $H_2^+$ ,  $HD^+$  or  $(D_2^+, (d^+p^+e)^+, (d^+p^+\mu^-)^+, (d^+d^+\mu^-)^+)$  as in muon catalysis. In general in heavy fermion systems we have to do with  $m_F \gtrsim m_\mu = 207 m_e$ . In this way  $a_F$  is an analogue of a Bohr radius

$$a_F = \varepsilon \left(\frac{m_e}{m_F}\right) a_B = \left(\frac{m_e}{\frac{m_F}{\varepsilon}}\right) a_B$$
 (6)

$$a_B = 0.5292 \cdot 10^{-10} \,\mathrm{m},\tag{7}$$

where  $\varepsilon$  is a dielectric constant of the material. Thus we can apply the theory known as mesomolecules theory simply putting in the place of  $m_{\mu}$  (a mass of a muon) an effective mass (from the point of view of the tunnel effect) of a heavy fermion divided by the dielectric constant of the material  $-\frac{m_F}{\varepsilon}$  (see Ref. [1]). In this way we can consider bound states of two deuterons or proton and deuteron bind by a quasiparticle (a heavy fermion) in a solid state lattice. This bond is very similar to ordinary chemical bond in  $H_2^+$  or  $(DH)^+$ . Moreover because of a relation (6) it is much more tight. Both nuclei are closer in the quasimolecule. Because of this a tunnel effect (through a Coulomb barriere), which will cause a nuclear reaction, is much more possible than in the case

of  $D_2^+$  or  $(DH)^+$ . According to Ref. [1] we get using Gamov theory of a tunnel effect:

$$B_F \simeq \exp\left(-\frac{2}{\hbar}(2Mq^2a_F)^{1/2}\right) \cong \exp\left(-K\sqrt{\frac{M\varepsilon}{m_F}}\right)$$
 (8)

 $(B_F \text{ is a probability of a tunnel effect})$ , where  $K \simeq 3 \div 3.3$ , M is a mass of a nucleus  $(d^+, p^+ \text{ or } t^+)$  or

$$B_F \simeq \exp\left(-K\sqrt{\frac{M}{m_e}}\cdot\sqrt{\frac{m_e\varepsilon}{m_F}}\right) = \left(\exp\left(-K\sqrt{\frac{M}{m_e}}\right)\right)^{\sqrt{\varepsilon m_e/m_F}}.$$
 (9)

It is easy to write (9) in terms of  $B_{\mu}$ —a probability of a muon catalysed nuclear fusion

$$B_F \simeq (B_\mu)^{\sqrt{\frac{\varepsilon m_\mu}{m_F}}}.$$
 (9a)

In this way we get a higher probability of a tunnel effect and a higher probability of a nuclear reaction. However we should take under consideration a different dielectric constant of a material with heavy fermions. In this way we get something which can be called a heavy fermion catalysis for low energy nuclear reactions. We can repeat all the considerations of Ref. [1] concerning muon catalysis. If the mass of a heavy fermion divided by a dielectric constant of the material is  $m_{\mu}$  the numerical results are exactly the same. Moreover we do not need any muon factory and some negative results of Ref. [1] are not applicable. We need only a heavy fermion system with an affinity for a hydrogen (a different dielectric constant of this material should be taken into account). Thus we should consider a material with a high affinity for hydrogen with heavy electrons. In that material we should have a high density of hydrogen storage. Thus we consider the following processes

$$d^{+} + d^{+} + F^{-} \to (d^{+}d^{+}F^{-})^{+}$$

$$d^{+} + t^{+} + F^{-} \to (d^{+}t^{+}F^{-})^{+}$$

$$d^{+} + p^{+} + F^{-} \to (d^{+}p^{+}F^{-})^{+}.$$
(10)

These three bodies processes can go via two stages

$$X^{+} + F^{-} \to (X^{+}F^{-})$$
  
 $(X^{+}F^{-}) + {X'}^{+} \to (X^{+}{X'}^{+}F^{-})$  (10a)

where  $X^+, X'^+ = p^+, d^+, t^+$ .

In those quasimolecular processes we get quasichemical bonds (quasimolecules) of  $d^+, t^+$  or  $p^+$ . Due to this we can expect higher rates of nuclear reactions

$$d^{+} + d^{+} \to \begin{cases} t^{+} + p^{+} + 4 \,\text{MeV} & -1\\ {}^{3}\text{He} + n + 3.3 \,\text{MeV} & -2\\ {}^{4}\text{He} + \gamma + 24 \,\text{MeV} & -3 \end{cases}$$
 (11)

coming to cold-fusion with heavy fermion catalysis.

Is it possible to realize this idea in practice? In order to realize it we should satisfy two conditions:

- 1) We should find a material with heavy fermions (as high mass as possible) and with a high affinity for hydrogen. Possibly as high as possible i.e. a hydrogen storage.
- 2) To find a condition for a work of this system (hydrogen storage + heavy fermion systems). Probably in a low temperature where we have to do with a high density of heavy fermions.

What kind of materials have we on the market? First of all we have heavy fermion superconductors:  $Ce Cu_2Si_2$ ,  $UPt_3$ ,  $U(Be_{1-x}Th_x)_{13}$  ( $0 \le x \le 1$ ),  $UPd_2Al_3$ ,  $UNi_2Al_3$ ,  $URu_2Si_2$ ,  $Ce Cu_2Ge_2$ ,  $Ce Rh_2Si_2$ ,  $Ce Ni_2Ge_2$ ,  $Ce In_3$ ,  $Th Cr_2Si_2$ ,  $Ce T In_3$  (T = Co, Rh, Ir),  $UGe_2$ ,  $Pu Co Ga_5$ .

Those materials are divided into two classes—the so-called Ce-based compounds and U-based compounds.

The effective mass of an electron is here several hundred times larger than a mass of a free electron due to strong electron correlations.

Some of those materials possess ferromagnetic or antiferromagnetic properties. The heavy fermion (heavy electron quasiparticle) is in general mixture of d-band or f-band electron with ordinary conduction electron. For example for  $\text{Ce Cu}_2\text{Si}_2$   $m_F \simeq 220m_e$ , for  $\text{UPt}_3$   $m_F \simeq 200m_e$ , for  $\text{UBe}_{13}$   $m_F \simeq 192m_e$  (see Ref. [3]).

The second group is a heavy fermion semiconductors group:  $Sm B_6$ ,  $Yb B_{12}$ ,  $Ce Bi_4Pt_3$ , Ce Ni Sm, Ce Rh Sb, U Ni Sm,  $Ce_3Sb_4Pt_3$ ,  $Ce Sb_4Au_3$ ,  $Ce Fe_4P_{12}$ , Ce Rh As,  $U_3Sb_4Pt_3$ ,  $U_3Sb_4Pt_3$ ,  $U Fe_4P_{12}$ , Fe Si.

They also have ferromagnetic properties.

The physical origin of an appearance of a large quasiparticle—a heavy electron—is the same as for the first group. For example for Fe Si,  $m_F \simeq 14 m_e$  (see Ref. [3]).

All of those materials are intermetallic compounds involving lantanides (rare earth elements) and actinides or Pd (palladium), Pt (platinium). It is very well known that rare earth elements, actinides, Pd, Pt, Ni and their intermetallic compounds possess high affinity for hydrogen. For example Y Ni<sub>2</sub>B<sub>2</sub>C (see [9]). Some of them are used as hydrogen storage: Pd (as Pd H<sub>0.6</sub>), La Ni<sub>5</sub> (as La Ni<sub>5</sub>H<sub>6</sub>), Mg<sub>2</sub>Ni (Mg<sub>2</sub>Ni H<sub>2</sub>). In brackets we give formulae for hydrides of those intermetallics (Ref. [4]). For example Pd can absorb 0.56 mass% of hydrogen and La Ni<sub>5</sub> 1.37. The unusual properties of palladium-hydrogen system has been mentioned (Ref. [4]). The hydrogen absorption in intermetallic compounds for lantanides and actinides has been reviewed in the last two points of Ref. [4]. Thus we should look for such materials among lantanides' and actinides' intermetallics (also for Pd and Pt). However in the case Pd H<sub>0.6</sub>  $m_F \approx 2 \div 3m_e$  which is quite small and maybe because of this cold fusion in palladium-hydrogen system is not effective. The Palladium Hydride is an ordinary low temperature superconductor with a reverse isotope effect (see Ref. [10]). The superconductivity for Pd H system has been observed by T. Skośkiewicz (see Ref. [11]).

Let us notice that quasimolecular processes (10) can be described by a very well developed quantum-mechanical formalism applied for meso-atoms and meso-molecules.

In this formalism we can calculate reaction rates calculating crosssections for those processes (see Ref. [1]). The interesting point (if this idea works) is to use practically energy from (11). From the third one it would be possible to get it via a cascade of ionization processes and pair creation. In this way due to pair creation of  $e^+e^-$  and afterwards electron-hole creation in semiconductors we can try to get an energy in some kind of a battery device. The same can be said for the first reaction of (11). In the case of the second one we can expect only a heat production.

Eventually we mention the following problem: the existence of a bound state of two nuclei and a quasiparticle. In the case of muon catalysis this problem has been solved (see Ref. [12]) and such a bound state really exists. The existence of the state has been confirmed in experiments (see Refs [12], [13]). Using the same formalism as in the approach of Ponomarev et al. we can prove the existence of the bound state in our case. Thus we get a quasichemical bond of two deuterons and a heavy fermion. The problem of a stickness of a muon which plagues a muon catalysis does not concern us for we have to do with many heavy fermions in a material. Thus we have to do with chemically assisted nuclear reactions.

It is worth to mention that an idea of screening of a Coulomb potential in low energy nuclear reactions by electrons in metals gives an enhancement of deuteron fusion reactions (see Ref. [14]).

Let us consider a fusion process in a hydrogen storage medium. First of all we should supply this medium with deuterium and tritium mixture ( $D_2$  and DT) or with pure deuterium ( $D_2$ ). In the medium we should determine a rate of  $d^+F^-$  "atom" production and to find a sign of the existence of those "atoms". Such an atom according to QM can be in excited state and emits (for absorbs) an electromagnetic radiation (a photon) of a frequency

$$h\nu_{nm} = E_m - E_n, \quad n < m \tag{12}$$

where

$$E_n = -\frac{\overline{R}_{\infty}}{n^2} \cdot \frac{1}{1 + \frac{m_{\rm F}}{M_{\rm D}}} \tag{13}$$

$$\overline{R}_{\infty} = \frac{m_F q^4}{32\pi^2 \varepsilon_0^2 \hbar^2 \varepsilon^2} \tag{14}$$

where  $M_{\rm D}$  is the mass of a nucleus of deuterium and q an elementary charge. We need  $d^+{\rm F}^-$  in a ground state n=1 and of course for l=0.

Let us consider Eqs (12)–(14). One gets

$$\nu_{nm}(m_{\rm F}, \varepsilon, M_{\rm D}) = \nu_{nm}({\rm H}) \frac{\left(1 + \frac{m_e}{m_p}\right)}{\left(1 + \frac{m_{\rm F}}{M_{\rm D}}\right)} \left(\frac{m_{\rm F}}{m_e}\right) \frac{1}{\varepsilon^2}$$
(15)

or

$$\lambda_{nm}(m_{\rm F}, \varepsilon, M_{\rm D}) = \lambda_{nm}({\rm H}) \frac{(1 + \frac{m_{\rm F}}{M_{\rm D}})}{(1 + \frac{m_e}{m_e})} \left(\frac{m_e}{m_{\rm F}}\right) \varepsilon^2$$
 (16)

where  $\nu_{nm}(m_{\rm F}, \varepsilon, M_{\rm D})$  means a frequency of a spectrum of  $d^+{\rm F}^-$  "atom",  $\nu_{nm}({\rm H})$  a frequency of a spectrum of hydrogen atom,  $\lambda_{nm}(m_{\rm F}, \varepsilon, M_{\rm D})$  and  $\lambda_{nm}({\rm H})$  the corresponding lengths and  $m_p$  a mass of a proton. Eqs (15)–(16) can be rewritten:

$$\nu_{nm}(m_{\rm F}, \varepsilon, M_{\rm D}) = \nu_{nm}({\rm H}) \frac{1.0005446 \, m_{\rm F}}{(1 + 2.7233 \times 10^{-4} \, m_{\rm F})\varepsilon^2}$$
 (15a)

$$\lambda_{nm}(m_{\rm F}, \varepsilon, M_{\rm D}) = \lambda_{nm}({\rm H}) \frac{0.999456(1 + 2.7233 \times 10^{-4} m_{\rm F})\varepsilon^2}{m_{\rm F}}$$
 (16a)

where now  $m_{\rm F}$  is measured in  $m_e$  units and we use values of  $M_{\rm D}$ ,  $m_p$ ,  $m_e$  from physical data. It is easy to see that usually  $\lambda_{nm}({\rm H}) > \lambda_{nm}(m_{\rm F}, \varepsilon, M_{\rm D})$ . In this way visual spectrum of hydrogen corresponds to UV spectrum of our  $d^+{\rm F}^-$  atom. Thus Paschen (n=3) or even Brackett (n=4), Pfund (n=5), Humphreys (n=6) spectral series correspond to visual or infrared spectral series of  $d^+{\rm F}^-$  atom. In a future experiment with a tunable laser radiation we should look for infrared spectral lines of  $d^+{\rm F}^-$  atom corresponding to higher spectral series  $(n \ge 4)$ . An emission or an absorption process is of an electric dipole nature, i.e. E1.

Moreover, from a practical point of view we should consider the following strategy. First of all we should fill our sample of a material with ordinary hydrogen and to look for the existence of  $p^+F^- = H^+F^-$  atom. The methodology is exactly the same as for  $d^+F^-$  atom. We are using a tunable laser for looking for an absorption spectrum of  $H^+F^-$ . Moreover, the spectrum will be a little different

$$\nu_{nm}(m_{\rm F},\varepsilon) = \nu_{nm}({\rm H}) \frac{\left(1 + \frac{m_e}{m_p}\right)}{\left(1 + \frac{m_{\rm F}}{m_p}\right)} \left(\frac{m_{\rm F}}{m_e}\right) \frac{1}{\varepsilon^2}$$
(17)

or

$$\lambda_{nm}(m_{\rm F},\varepsilon) = \lambda_{nm}({\rm H}) \frac{(1 + \frac{m_{\rm F}}{m_p})}{(1 + \frac{m_e}{m_p})} \left(\frac{m_e}{m_{\rm F}}\right) \varepsilon^2$$
 (18)

where  $\nu_{nm}(m_{\rm F}, \varepsilon)$  means a frequency of a spectrum of H<sup>+</sup>F<sup>-</sup> "atom",  $\lambda_{nm}(m_{\rm F}, \varepsilon)$  the corresponding length.

Equations (17)–(18) can be rewritten:

$$\nu_{nm}(m_{\rm F}, \varepsilon) = \nu_{nm}(H) \frac{1}{\varepsilon^2} \frac{1.0005446 \, m_{\rm F}}{(1 + 5.446 \times 10^{-4} \, m_{\rm F})}$$
(17a)

$$\lambda_{nm}(m_{\rm F}, \varepsilon) = \lambda_{nm}({\rm H})\varepsilon^2 \frac{0.999456(1 + 5.446 \times 10^{-4} m_{\rm F})}{m_{\rm F}}$$
 (18a)

where  $m_F$  is measured in  $m_e$  units.

It is easy to see that

$$\lambda_{nm}(H) > \lambda_{nm}(m_{\rm F}, \varepsilon) > \lambda_{nm}(m_{\rm F}, \varepsilon, M_{\rm D}).$$

As in the case of  $d^+F^-$  atom we should look for n > 3 spectral series to be in visual or infrared region.

Let us notice that in the case of  $H^+F^-$  and  $d^+F^-$  "atoms" we can expect also so-called Rydbergs atoms as in the case of exitons (as in  $Cu_2O$  case), i.e. in a very high quantum number n. The absorption spectrum of those "atoms" would not be Lorentzian (not symmetric). The spectrum will be distorted due to an overall absorption and a shape will be described by a Fano curve.

The next step is a formation of an analogue  $H_2^+$  (ionized hydrogen molecule), i.e.  $p^+p^+F^- = H^+H^+F^-$ . In the case of muon catalysis there are some resonances which allow us to form a  $\mu^-d^+d^+$  molecule. In our case such resonance can appear for  $F^-H^+H^+$  or  $F^-d^+d^+$  quasimolecules. Thus we should find some signals for an existence of such a quasimolecule in a piece of a material of heavy fermion systems filled with an ordinary hydrogen. This can be achieved only via spectroscopy of such a molecule.

Let us sketch some properties of such a molecule from the point of view of QM (Quantum Mechanics). A Schrödinger equation for such a three body system is as follows

$$H\psi = E\psi \tag{19}$$

where

$$H = -\frac{\hbar^2}{2m_{\rm F}} \vec{\nabla}^2 + \frac{q^2}{4\pi\varepsilon_0\varepsilon} \left(\frac{Z_A}{r_a} + \frac{Z_B}{r_b}\right). \tag{20}$$

Usually we suppose  $Z_A = Z_B$ . In this approach we neglect a motion of nuclei and consider a motion of heavy electron in a two-fixed-center potential. In atomic units Eq. (19) can be rewritten

$$\left(\vec{\nabla}^2 + 2\left(\frac{\widetilde{Z}_A}{r_a} + \frac{\widetilde{Z}_B}{r_b}\right) + 2\widetilde{E}\right)\psi = 0 \tag{21}$$

where

$$\widetilde{Z}_A = \frac{m_F}{\varepsilon} \cdot Z_A, \quad \widetilde{Z}_B = \frac{m_F}{\varepsilon} \cdot Z_B, \quad \widetilde{E} = m_F E.$$
 (22)

 $m_{\rm F}$  is measured in  $m_e$  units.  $r_a$  and  $r_b$  are distances of an heavy electron for two nuclei. According to Ref. [15], Eq. (21) can be separated in prolate-spheroidal coordinates

$$\xi = (r_a + r_b)/R, \quad 1 \le \xi \le \infty,$$
  

$$\eta = (r_a - r_b)/R, \quad -1 \le \eta \le 1,$$
(23)

$$Q_1 = R(\widetilde{Z}_A - \widetilde{Z}_B) \tag{24}$$

$$Q_2 = R(\widetilde{Z}_A + \widetilde{Z}_B)$$

$$0 \le \varphi \le 2\pi.$$
(25)

 $0 \leq \varphi \leq 2\pi$ .

 $\varphi$  is an azimuth angle, R is the distance between nuclei,

$$\psi(\xi, \eta, \varphi) = \Lambda(\xi)M(\eta, \varphi) = \Lambda(\xi)G(\eta)e^{\pm im\varphi}$$
(26)

(see Ref. [15]). One gets

$$\left[\frac{\partial}{\partial \eta}\left((1-\eta^2)\frac{\partial}{\partial \eta}\right) - \frac{m^2}{1-\eta^2} - p^2\eta^2 - Q_1\eta - A\right]M(\eta,\varphi) = 0$$
 (27)

$$\left[\frac{\partial}{\partial \xi} \left( (\xi^2 - 1) \frac{\partial}{\partial \xi} \right) - \frac{m^2}{\xi^2 - 1} - p^2 \xi^2 - Q_2 \xi + A \right] \Lambda(\xi) = 0, \tag{28}$$

A is a separation constant. Thus we reduce the problem  $H^+H^+F^-$  to the ordinary  $H_2^+$  problem with some rescaling. If we denote a solution of Eq. (21) by  $\Psi_{\widetilde{Z}_A,\widetilde{Z}_B,\widetilde{E}}(\xi,\eta,\varphi)$  we get for  $H^+H^+F^-$ ,  $\Psi_{m_F,m_F,m_FE}(\xi,\eta,\varphi)$ , where E is an eigenvalue of an energy for  $H^+H^+F^-$  molecule. According to Ref. [15] the solution of Eq. (27) should be expanded into spherical harmonics

$$M(\eta, \varphi) = \sum_{k=m}^{\infty} f_m^k Y_k^m(\eta, \varphi)$$
 (29a)

$$\Lambda(\xi) = e^{-p(\xi-1)} [p(\xi-1)]^{m/2} \sum_{n=m/2}^{\infty} C_{n-(m/2)} \mathcal{L}_{n-(m/2)}^{m} [2p(\xi-1)].$$
 (29b)

For A and  $p^2$  we have

$$\lim_{R \to 0} A = -l(l+1), \quad \lim_{R \to 0} p^2 = 0 \tag{30}$$

(a united atom limit),  $\mathcal{L}_k^m(x)$  are Laguerre polynomials.

Quantum numbers n, l, m are good quantum numbers only in the limit of a united atom (we are using them). In general only m is a good quantum number

$$\widetilde{E} = \widetilde{E}_{\text{elec}} = -2 \frac{p^2}{R^2} \,,$$
 (31)

 $p^2$  depends also on  $\widetilde{Z}_A$  and  $\widetilde{Z}_B$ . In our case  $\widetilde{Z}_A = \widetilde{Z}_B = m_{\rm F}$ . There are a lot of computer programs which can solve equations for any  $\widetilde{Z}_A = \widetilde{Z}_B = m_{\rm F}$  getting  $\widetilde{E}$  which is equal to electron energy (see Ref. [15] and references therein). Moreover, we should add an energy of nuclei equal to  $\frac{1}{\varepsilon R}$  and calculate the minimum with respect to R. This gives us a ground state energy. We should remember that we have to do with symmetric and antisymmetric states. The ground state of  $H_2^+$  is denoted by  $X^2 \Sigma_g^+$  or  $1s\sigma_g$  and is symmetric. The first excited state  $A^2 \Sigma_u^+$  or  $2p\sigma_u$  is antisymmetric. Thus we can expect similar states for  $H^+H^+F^-$  molecule but rescaled (also  $^2\Pi_u$  or  $^2\Pi_g$ ) by  $m_{\rm F}$  and  $\varepsilon$ . This means we should look for more energetic spectrum using a tunable laser method in order to prove the existence of  $H^+H^+F^-$ .

Afterwards we should consider a  $d^+F^-d^+$  or  $d^+F^-t^+$  molecule formation. The most important feature is an interaction between an atom  $d^+F^-$  (dF) and  $d^+$  or  $t^+$ . We can suppose it is a harmonic potential or a Morse potential and similarly as in muon

catalyzed fusion we expect  $(ddF)^+$  for K=1, v=1, where K is an angular momentum quantum number for a molecule and v is a vibrational number (see Ref. [16]). In the case of  $(dFt)^+$  we can employ similar mechanism based on E1 transition. We need  $(dFd)^+$  and  $(dFt)^+$  in a ground state. In the ground state a tunnel effect causes a fusion very efficiently. For a muon catalyzed fusion we have  $10^{-12}$  s for a nuclear fusion. Using formulas (9) and (9a) we get

$$10^{-12\sqrt{\frac{m_{\rm F}}{\varepsilon m_{\mu}}}}$$
 s

which is smaller than  $10^{-12}$  s (for a muon catalyzed fusion) if  $\frac{m_{\rm F}}{\varepsilon} > m_{\mu}$ . Let us estimate a rate of a fusion in our hydrogen storage medium per a unit of volume.

One gets

$$Y = \varphi \cdot \lambda_{(dF)} \lambda_{(dFd)} + B_F \cdot \rho_H \tag{32}$$

where  $\varphi$  is a density of D in a hydrogen storage normalized to the density of a liquid hydrogen ( $\rho_{\rm H}$  is a density of a liquid hydrogen measured in atoms on cm<sup>3</sup>,  $\rho_{\rm H} = 4.25 \times 10^{22} \, {\rm atoms/cm^3}$ ). This value can be greater than one.

 $\lambda_{(dF)}$ ,  $\lambda_{(dFd)^+}$  are respectively probabilities of an atom (dF) formation in a ground state and quasi-molecules formation  $(dFd)^+$ .  $B_F$  is a probability of a tunnel effect (see similar formulas for a muon catalyzed fusion Ref. [17]). We neglect an existence of tritium in a sample.

Let us apply Eq. (15) in the case of reactions (11). One gets

$$e_i = \varphi \lambda_{(dF)} \lambda_{(dFd)^+} B_F \rho_H B_i E_i, \quad i = 1, 2, 3, \tag{33}$$

where  $e_i$  is an energy production in one second per the unit of volume for three reactions in (11).  $E_i$  is an energy for a reaction number i,  $E_1 = 4 \,\text{MeV}$ ,  $E_2 = 3.3 \,\text{MeV}$ ,  $E_3 = 24 \,\text{MeV}$ .  $B_i$ , i = 1, 2, 3, are branching ratios of these reactions:  $B_1 \simeq B_2 \simeq 50\%$  and  $B_3$  is very small, i.e.  $B_3 \simeq 10^{-6}$ . From practical point of view 1 and 3 are very important for they are "aneutronic" reactions. They produce charged particles and for this they can be a source of an electrical energy without conversion from thermal to electrical energy. For the process of an energy conversion is more efficient.

One can criticize our approach to cold fusion, i.e. a presence of a strong "heavy electron" screening of the Coulomb barrier which would prevent cold fusion. One argues the physical basis of the claim of strong electron screening on a length scale much less than an angström is false.

This claim is based on the following reasoning. In the crystal with "heavy electron" band we have periodic band energy

$$E(\vec{k}) = E_0 - \sum_{\vec{M} \neq 0} H(\vec{M}) \cos(\vec{k} \cdot \vec{M})$$
 (34)

where  $H(\vec{M})$  is the Hamiltonian for the electron to go from one crystal cell to another, where  $\vec{M}$  is a lattice vector connecting two cells. If matrix elements of the Hamiltonian

 $|H(\vec{M})| \ll 1 \, \mathrm{eV}$  the electron behaves as heavy for its velocity is small

$$\vec{v}(\vec{k}) = \frac{1}{\hbar} \left( \frac{\partial E}{\partial \vec{k}} \right) = \frac{1}{\hbar} \sum_{\vec{M} \neq 0} \vec{M} H(\vec{M}) \sin(\vec{k}\vec{M}). \tag{35}$$

Those electrons are trapped in a localized Wannier state which can have wide spatial dispersion. In this way the bound deuteron–electron wave function can be of order  $\sim 1\,\text{Å}$  size as in the vacuum which makes impossible to screen the Coulomb barrier and afterwards a bigger probability of a tunnel effect.

Moreover, we can make a localized Wannier state narrower making "heavy electron" band localized, which is possible in some mentioned materials, i.e. in materials which are superconductors (heavy fermion superconductors). In this way we have to do with so-called CMNS (condensed matter nuclear science).

Thus the mentioned mechanism can work and only the experiment can settle the controversy.

How to design an experiment? First of all we should choose a hydrogen storage with heavy fermions and afterwards fill it with deuterium. (It is reasonable first to fill a sample of a hydrogen storage with heavy fermion material with an ordinary hydrogen H, in order to find which of them (i.e. materials) are able to form quasiatoms  $H^+F^-$ . This can be achieved by spectroscopic methods using a tunable laser. Only such materials should be filled afterwards with deuterium.) Then we should look for an absorption spectrum of  $(d^+F^-)$  (see Eqs (12)–(14)) to be sure that in our piece of material filled with  $D_2$  there is an interaction between  $d^+$  and  $F^-$ . This is a first step of the experiment. If we confirm this step we can go to the second step of the experiment. Now we should look for some products of low energy nuclear reactions, i.e. for  $p^+$  (protons),  $\gamma$ —photons and n (neutrons). If we detect them on the level higher than the background radiation we can be sure that the mechanism works. We should work with several materials by trial and error method.

Thus we should use a tunable laser to obtain the required frequency of light (Eqs (12)–(13)) to observe an absorption and emission of photons and detectors of photons. According to a common practice for such an experiment we are required to put a device with deuterium inside a calorimeter (e.g. flow-type calorimeter—SRI International flow calorimeter) in order to measure heat production. The energetic particles can be detected by CR-39, a plastic that suffers local damage by passage of charge particles or neutrons being a track detectors (solid-state nuclear track detectors). We can also observe tracks on X-ray films. The detectors should record the history of nuclear emission from an experiment and signal-to-noise ratios. The important point is to keep out of a possible chemical reaction heat sources, first of all to keep out of a possible reaction  $2D_2 + O_2 \rightarrow 2D_2O$  which could be a source of undesired heat. For we have to do with many intermetallic materials, we should also keep out of phase transitions among several phases which can be a source or sink of heat.

The interesting point in these investigations is a problem of thermodynamical description of a device: 1) a piece of material with heavy fermion system, 2) a flow of

deuterium in the calorimeter. It seems that we should use non-equilibrium thermodynamics. Moreover, it is natural to consider non-equilibrium (irreversible) thermodynamics close to equilibrium. Such thermodynamics uses Onsager relations and a principle of minimal entropy production. Thus we should identify flows and thermodynamic forces and consider a possible free energy (enthalpy) production locally. In our case we have to do with chemical-like reactions as in Eq. (11). Considering Eq. (11) as a chemical reaction we get

$$J_i = \frac{\varphi}{N_A} \lambda_{(dF)} \lambda_{(dFd)^+} B_F \rho_H B_i$$

we should also add an additional reaction

$$d^{+} + d^{+} \to d^{+} + d^{+} \tag{36}$$

and

$$J_4 = \frac{\varphi}{N_A} \left( 1 - \lambda_{(dF)} \lambda_{(dFd)^+} B_F \right) \rho_H. \tag{37}$$

Thus we define functions of a progress of reactions  $J_j$ , j = 1, 2, 3, 4.  $N_A$  is the Avogadro number.

Let us define

$$A_1 \to d^+, \quad A_2 \to d^+, \quad A_3 \to t^+, \quad A_4 \to p^+,$$
  
 $A_5 \to {}^3\text{He}, \quad A_6 \to n, \quad A_7 \to {}^4\text{He}, \quad A_8 \to \gamma.$ 

Thus we have 8 components in four reactions.

We define stechiometric coefficients a j component of i reaction  $\xi_{ij}$ . We get

$$\xi_{ij} = \begin{pmatrix} -1 & -1 & 1 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 & 1 & 1 & 0 & 0 \\ -1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$
(38)

We have

$$\sum_{i=1}^{8} \xi_{ij} A_i = 0, \quad j = 1, 2, 3, 4.$$
(39)

Let us denote by  $M_i$  a moll mass of the component  $A_i$ . Thus we have

$$M_1=M_2=M_{d^+}, \quad M_3=M_{t^+}, \quad M_4=M_{p^+}, \ M_5=M_{^3{
m He}}, \quad M_6=M_n, \quad M_7=M_{^4{
m He}}, \quad M_8=M_{\gamma}.$$

A typical conservation law known in chemistry (a conservation of substance) can be written only as

$$\sum_{i=1}^{8} \xi_{ij} M_i \approx 0 \tag{40}$$

for we have an energy production and this has an influence on the total mass.

We get a source term due to chemical reactions

$$M_i \sum_{j} \xi_{ij} J_j. \tag{41}$$

Let us define a balance equation for the i-th component

$$\frac{\partial \rho_j}{\partial t} = -\operatorname{div}(\rho_j \vec{v}_i) - \operatorname{div} \vec{\jmath}_j + M_i \sum_i \xi_{ji} J_i, \tag{42}$$

where  $\rho_j$ ,  $\vec{v}_j$  and  $\vec{\jmath}_j$  are density, velocity and diffusion flux of the j-th component. It is easy to see that for j=1,2 we have the same balance of deuterium, for j=8  $\vec{v}_j=0$ .

One can derive the following equation for an internal energy density

$$\rho \frac{du}{dt} = -\operatorname{div}(\rho u \vec{v}) - p \operatorname{div} \vec{v} + \frac{\rho}{N_A} \sum_{i=1}^{3} e_i.$$
(43)

For a density of an entropy one gets

$$\rho \frac{ds}{dt} = -\operatorname{div}\left(\frac{1}{T}\left(\rho u\vec{v} - \sum_{\substack{i=1\\i\neq 2}}^{8} \mu_i \vec{\jmath}_i\right)\right) - \frac{\rho u}{T^2} \vec{v} \cdot \vec{\nabla}T - \sum_{\substack{i=1\\i\neq 2}}^{8} \vec{\jmath}_i \cdot \vec{\nabla}\left(\frac{\mu_i}{T}\right) + \frac{1}{T} \sum_{j=1}^{4} \overline{A}_j J_j.$$
(44)

where

$$\overline{A}_j = \sum_{\substack{i=1\\i\neq 2}}^8 \mu_i \xi_{ij} M_i$$

and  $\mu_i$  is a chemical potential of the *i*-th component. This is basically a thermodynamics of our system.

Moreover, we are interested in a free energy production. One gets for f

$$\rho f = \rho(u - Ts)$$

$$\rho \frac{df}{dt} = -\operatorname{div}(\rho u \vec{v}) + T\operatorname{div}\left(\frac{1}{T}\left(\rho u \vec{v} - \sum_{\substack{i=1\\i\neq 2}}^{8} \mu_i \vec{\jmath}_i\right)\right) + \frac{\rho u}{T} \vec{v} \cdot \vec{\nabla} T$$

$$(45)$$

$$+ T \sum_{\substack{i=1\\i\neq 2}}^{8} \vec{j}_{i} \vec{\nabla} \left(\frac{\mu_{i}}{T}\right) - \sum_{j=1}^{4} \overline{A}_{j} J_{j} - p \operatorname{div} \vec{v} + \frac{\rho}{N_{A}} \sum_{i=1}^{3} e_{i}.$$
 (46)

We can also consider a density of a free enthalpy production:

$$g = u - Ts + \frac{pV}{\rho} \tag{47}$$

getting

$$\rho \frac{dg}{dt} = \rho \frac{df}{dt} + \rho \frac{d}{dt} \left(\frac{pV}{\rho}\right) \tag{48}$$

where p is a pressure, V—a volume,  $\vec{v}$ —a velocity, T—a temperature,  $\rho$ —density,  $\vec{j_i}$ —a diffusion flux,  $\overline{A_i}$ —a chemical affinity.

Let us notice that g is important for isothermo-isobaric processes and f for isothermo-isochoric processes

$$\vec{j_i} = -D_i \vec{\nabla} C_i \tag{49}$$

where  $D_i$  is a diffusion constant and  $c_i$  are concentration.

Eventually let us define two important functions  $\Phi$  and  $\Psi$ :

$$\Phi = \rho u \vec{v} \cdot \vec{\nabla} \left(\frac{1}{T}\right) - \sum_{\substack{j=1\\j\neq 2}}^{8} \vec{\jmath}_j \cdot \vec{\nabla} \left(\frac{\mu_j}{T}\right) + \frac{1}{T} \sum_{j=1}^{4} A_j J_j$$
 (50)

$$\Psi = T\Phi \tag{51}$$

 $\Phi$  is an entropy production function and  $\Psi$  is a dissipation function. We neglect a heat conduction in a sample supposing it is small in size.

Let us consider Eq. (50) in more details. One gets

$$\Phi = \rho u \vec{v} \cdot \vec{\nabla} \left( \frac{1}{T} \right) + D_{d^{+}} \vec{\nabla} C_{d^{+}} \vec{\nabla} \left( \frac{\mu_{d^{+}}}{T} \right) + D_{t^{+}} \vec{\nabla} C_{t^{+}} \cdot \vec{\nabla} \left( \frac{\mu_{t^{+}}}{T} \right) 
+ D_{p^{+}} \vec{\nabla} C_{p^{+}} \cdot \vec{\nabla} \left( \frac{\mu_{p^{+}}}{T} \right) + D_{3\text{He}} \vec{\nabla} C_{3\text{He}} \vec{\nabla} \left( \frac{\mu_{3\text{He}}}{T} \right) + D_{n} \vec{\nabla} C_{n} \cdot \vec{\nabla} \left( \frac{\mu_{n}}{T} \right) 
+ D_{4\text{He}} \vec{\nabla} C_{4\text{He}} \vec{\nabla} \left( \frac{\mu_{4\text{He}}}{T} \right) + D_{\gamma} \vec{\nabla} C_{\gamma} \cdot \vec{\nabla} \left( \frac{\mu_{\gamma}}{T} \right) + \frac{\varphi B_{F} \rho_{H} \lambda_{(dF)} \lambda_{(dFd)^{+}}}{T N_{A}}$$

$$\cdot \left[ B_{1} \left( \mu_{t^{+}} M_{t^{+}} + \mu_{p^{+}} M_{p^{+}} \right) + B_{2} \left( \mu_{3\text{He}} M_{3\text{He}} + \mu_{n} M_{n} \right) \right] 
+ B_{3} \left( \mu_{4\text{He}} M_{4\text{He}} + \mu_{\gamma} M_{\gamma} \right) - 2\mu_{d^{+}} M_{d^{+}}$$
(52)

where  $\mu, M, D, C$  are respectively chemical potentials, moll mass, coefficients of diffusion and concentrations of all components, i.e.  $d^+, t^+, p^+, n$ ,  ${}^3\text{He}$ ,  ${}^4\text{He}$  and  $\gamma$ .

The general principle of a nonequilibrium thermodynamics, formulated by Onsager and Prigogine, consists in a minimal entropy production  $\int\!\int\!\int_V\Phi\,dv=$  min. This is satisfied in a stationary case. In this way we go to the variational principle

$$\delta \iiint_{V} \Phi \, dv = 0 \tag{53}$$

where a variation is taken with respect to all mechanical, thermodynamical and chemical quantities. In particular with respect to  $T, \rho, \vec{v}, u, C_{d^+}, \mu_{d^+}, C_{t^+}, \mu_{t^+}, C_{p^+}, \mu_{p^+},$ 

 $C_{^{3}\text{He}}, \mu_{^{3}\text{He}}, C_n, \mu_n, C_{^{4}\text{He}}, \mu_{^{4}\text{He}}, C_{\gamma}, \mu_{\gamma}, \varphi$  established stationary boundary conditions for all quantities.

The variational problem can be written in a form of a system of partial differential equations for every function in the following way:

$$\vec{\nabla} \frac{\partial \Phi}{\partial \vec{\nabla}(\frac{1}{T})} - \frac{\partial \Phi}{\partial (\frac{1}{T})} = 0 \qquad \vec{\nabla} \frac{\partial \Phi}{\partial \vec{\nabla} \mu} - \frac{\partial \Phi}{\partial \mu} = 0$$

$$\vec{\nabla} \frac{\partial \Phi}{\partial \vec{\nabla} C} - \frac{\partial \Phi}{\partial C} = 0 \qquad \vec{\nabla} \frac{\partial \Phi}{\partial \vec{\nabla} \rho} - \frac{\partial \Phi}{\partial \rho} = 0$$

$$\vec{\nabla} \frac{\partial \Phi}{\partial \vec{\nabla} u} - \frac{\partial \Phi}{\partial u} = 0 \qquad \text{etc.}$$
(54)

$$\vec{\nabla}(\rho u \vec{v}) + \operatorname{div}\left(D_{d^{+}} \vec{\nabla} C_{d^{+}} \mu_{d^{+}} + D_{t^{+}} \vec{\nabla} C_{t^{+}} \mu_{t^{+}} + D_{p^{+}} \vec{\nabla} C_{p^{+}} \mu_{p^{+}} \right) \\
+ D_{{}^{3}\text{He}} \vec{\nabla} C_{{}^{3}\text{He}} \mu_{{}^{3}\text{He}} + D_{n} \vec{\nabla} C_{n} \mu_{n} + D_{{}^{4}\text{He}} \vec{\nabla} C_{{}^{4}\text{He}} \mu_{{}^{4}\text{He}} + D_{\gamma} \vec{\nabla} C_{\gamma} \mu_{\gamma}\right) \\
- \left(D_{d^{+}} \vec{\nabla} C_{d^{+}} \cdot \vec{\nabla} \mu_{d^{+}} + D_{t^{+}} \vec{\nabla} C_{t^{+}} \cdot \vec{\nabla} \mu_{t^{+}} + D_{p^{+}} \vec{\nabla} C_{p^{+}} \cdot \vec{\nabla} \mu_{p^{+}} \right) \\
+ D_{{}^{3}\text{He}} \vec{\nabla} C_{{}^{3}\text{He}} \cdot \vec{\nabla} \mu_{{}^{3}\text{He}} + D_{n} \vec{\nabla} C_{n} \cdot \vec{\nabla} \mu_{n} + D_{{}^{4}\text{He}} \vec{\nabla} C_{{}^{4}\text{He}} \cdot \vec{\nabla} \mu_{{}^{4}\text{He}} \\
+ D_{\gamma} \vec{\nabla} C_{\gamma} \cdot \vec{\nabla} \mu_{\gamma}\right) - \frac{\varphi B_{F} \rho_{H} \lambda_{(dF)} \lambda_{(dFd)^{+}}}{N_{A}} \cdot \left[B_{1}\left(\mu_{t^{+}} M_{t^{+}} + \mu_{p^{+}} M_{p^{+}}\right) \\
+ B_{2}\left(\mu_{{}^{3}\text{He}} M_{{}^{3}\text{He}} + \mu_{n} M_{n}\right) + B_{3}\left(\mu_{{}^{4}\text{He}} M_{{}^{4}\text{He}} + \mu_{\gamma} M_{\gamma}\right) - 2\mu_{d^{+}} M_{d^{+}}\right] = 0$$
(55)

$$\vec{\nabla} \frac{\partial \Phi}{\partial \vec{\nabla} \mu_{d^{+}}} - \frac{\partial \Phi}{\partial \mu_{d^{+}}} = 0 \tag{56}$$

$$\operatorname{div}\left(\frac{D_{d^{+}}}{T}\vec{\nabla}C_{d^{+}}\right) - D_{d^{+}}\vec{\nabla}\left(\frac{1}{T}\right)\vec{\nabla}C_{d^{+}} + \frac{2M_{d^{+}}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda(dFd)^{+}}{TN_{A}} = 0$$
 (57)

and for remaining concentrations

$$\operatorname{div}\left(\frac{D_{t^{+}}}{T}\vec{\nabla}C_{t^{+}}\right) - D_{t^{+}}\vec{\nabla}\left(\frac{1}{T}\right)\vec{\nabla}C_{t^{+}} - \frac{B_{1}M_{t^{+}}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda_{(dFd)^{+}}}{TN_{A}} = 0 \qquad (58)$$

$$\operatorname{div}\left(\frac{D_{p^{+}}}{T}\vec{\nabla}C_{p^{+}}\right) - D_{p^{+}}\vec{\nabla}\left(\frac{1}{T}\right)\vec{\nabla}C_{p^{+}} - \frac{B_{1}M_{p^{+}}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda_{(dFd)^{+}}}{TN_{A}} = 0 \quad (59)$$

$$\operatorname{div}\left(\frac{D_{^{3}\mathrm{He}}}{T} \vec{\nabla} C D_{^{3}\mathrm{He}}\right) - D_{^{3}\mathrm{He}} \vec{\nabla}\left(\frac{1}{T}\right) \vec{\nabla} C_{^{3}\mathrm{He}} - \frac{B_{2} M_{^{3}\mathrm{He}} \varphi B_{F} \rho_{H} \lambda_{(dF)} \lambda_{(dFd)^{+}}}{T N_{A}} = 0 (60)$$

$$\operatorname{div}\left(\frac{D_{^{4}\text{He}}}{T}\vec{\nabla}CD_{^{4}\text{He}}\right) - D_{^{4}\text{He}}\vec{\nabla}\left(\frac{1}{T}\right)\vec{\nabla}C_{^{4}\text{He}} - \frac{B_{3}M_{^{4}\text{He}}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda_{(dFd)^{+}}}{TN_{A}} = 0 (61)$$

$$\operatorname{div}\left(\frac{D_n}{T}\vec{\nabla}C_n\right) - D_n\vec{\nabla}\left(\frac{1}{T}\right)\vec{\nabla}C_n - \frac{B_2M_n\varphi B_F\rho_H\lambda_{(dF)}\lambda_{(dFd)^+}}{TN_A} = 0 \tag{62}$$

$$\operatorname{div}\left(\frac{D_{\gamma}}{T}\vec{\nabla}C_{\gamma}\right) - D_{\gamma}\vec{\nabla}\left(\frac{1}{T}\right)\vec{\nabla}C_{\gamma} - \frac{B_{3}M_{\gamma}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda_{(dFd)^{+}}}{TN_{A}} = 0.$$
 (63)

For chemical potentials one gets

$$\operatorname{div}\left(D_{d^{+}}\vec{\nabla}\left(\frac{\mu_{d^{+}}}{T}\right)\right) = 0\tag{64}$$

$$\operatorname{div}\left(D_{t^{+}}\vec{\nabla}\left(\frac{\mu_{t^{+}}}{T}\right)\right) = 0\tag{65}$$

$$\operatorname{div}\left(D_{p^{+}}\vec{\nabla}\left(\frac{\mu_{p^{+}}}{T}\right)\right) = 0 \tag{66}$$

$$\operatorname{div}\left(D_{{}^{3}\operatorname{He}}\vec{\nabla}\left(\frac{\mu^{{}^{3}\operatorname{He}}}{T}\right)\right) = 0 \tag{67}$$

$$\operatorname{div}\left(D_n\vec{\nabla}\left(\frac{\mu_n}{T}\right)\right) = 0\tag{68}$$

$$\operatorname{div}\left(D_{^{4}\!\mathrm{He}}\vec{\nabla}\left(\frac{\mu_{^{4}\!\mathrm{He}}}{T}\right)\right) = 0 \tag{69}$$

$$\operatorname{div}\left(D_{\gamma}\vec{\nabla}\left(\frac{\mu_{\gamma}}{T}\right)\right) = 0,\tag{70}$$

for a velocity one gets

$$\rho u \vec{\nabla} \left( \frac{1}{T} \right) = 0. \tag{71}$$

It means  $T=\mathrm{const.}$  For a parameter  $\varphi$  one gets

$$B_{1}(\mu_{t+}M_{t+} + \mu_{p+}M_{p+}) + B_{2}(\mu_{^{3}\text{He}}M_{^{3}\text{He}} + \mu_{n}M_{n}) + B_{3}(\mu_{^{4}\text{He}}M_{^{4}\text{He}} + \mu_{\gamma}M_{\gamma}) = 2\mu_{d+}M_{d+},$$
 (72)

which is a constraint for chemical potentials.

Variations with respect to  $\rho$  and u do not give us any equations. They are satisfied identically for  $T=\mathrm{const.}$ 

We should supply all the equations with boundary data on a boundary of a sample V. This depends on the shape of the sample.

For concentrations one gets after some simplifications

$$D_{d^{+}} \vec{\nabla}^{2} C_{d^{+}} + \frac{2M_{d^{+}} \varphi B_{F} \rho_{H} \lambda_{(dF)} \lambda_{(dFd)^{+}}}{N_{A}} = 0$$
 (73)

$$D_{t+}\vec{\nabla}^{2}C_{t+} - \frac{B_{1}M_{t+}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda_{(dFd)+}}{N_{A}} = 0$$
 (74)

$$D_{p^{+}} \vec{\nabla}^{2} C_{p^{+}} - \frac{B_{1} M_{p^{+}} \varphi B_{F} \rho_{H} \lambda_{(dF)} \lambda_{(dFd)^{+}}}{N_{A}} = 0$$
 (75)

$$D_{^{3}\text{He}}\vec{\nabla}^{2}C_{^{3}\text{He}} - \frac{B_{2}M_{^{3}\text{He}}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda_{(dFd)^{+}}}{N_{A}} = 0$$
 (76)

$$D_{\rm ^{4}He}\vec{\nabla}^{2}C_{\rm ^{4}He} - \frac{B_{3}M_{\rm ^{4}He}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda_{(dFd)^{+}}}{N_{A}} = 0$$
 (77)

$$D_n \vec{\nabla}^2 C_n - \frac{B_2 M_n \varphi B_F \rho_H \lambda_{(dF)} \lambda_{(dFd)^+}}{N_A} = 0$$
 (78)

$$D_{\gamma}\vec{\nabla}^{2}C_{\gamma} - \frac{B_{3}M_{\gamma}\varphi B_{F}\rho_{H}\lambda_{(dF)}\lambda_{(dFd)^{+}}}{N_{A}} = 0.$$
 (79)

For chemical potentials simply

$$\vec{\nabla}^2 \mu_{d^+} = \vec{\nabla}^2 \mu_{t^+} = \vec{\nabla}^2 \mu_{p^+} = \vec{\nabla}^2 \mu_{^3\text{He}} = \vec{\nabla}^2 \mu_n = \vec{\nabla}^2 \mu_{^4\text{He}} = \vec{\nabla}^2 \mu_{\gamma} = 0.$$
 (80)

Eqs (73–79) can be simply written as

$$\vec{\nabla}^2 C_i = \kappa K_i \tag{81}$$

where

$$\kappa = \frac{\varphi B_F \rho_H \lambda_{(dF)} \lambda_{(dFd)^+}}{N_A} \tag{82}$$

and  $i = d^+, t^+, p^+, {}^{3}\!\text{He}, {}^{4}\!\text{He}, n, \gamma,$ 

$$K_{d^{+}} = -\frac{2M_{d^{+}}}{D_{d^{+}}} \tag{83a}$$

$$K_{t^{+}} = \frac{B_1 M_{t^{+}}}{D_{t^{+}}} \tag{83b}$$

$$K_{p^{+}} = \frac{B_{1}M_{p^{+}}}{D_{p^{+}}} \tag{83c}$$

$$K_{\rm ^3He} = \frac{B_2 M_{\rm ^3He}}{D_{\rm ^3He}}$$
 (83d)

$$K_{\rm ^{4}He} = \frac{B_3 M_{\rm ^{4}He}}{D_{\rm ^{4}He}}$$
 (83e)

$$K_n = \frac{B_2 M_n}{D_n} \tag{83f}$$

$$K_{\gamma} = \frac{B_3 M_{\gamma}}{D_{\gamma}} \tag{83g}$$

We suppose that  $D_i$  are constant (coefficients of diffusion).

For chemical potentials satisfy Laplace equations the constraint (72) really means a constraint on a boundary data for those equations.

We put a solution of a variation problem to the equation (46) to get a free energy production. The important point is to calculate the second variation in order to check if we have to do with a minimum.

Thus one gets

$$\rho \frac{df}{dt} = -\operatorname{div}(\rho u \vec{v})$$

$$+ T \operatorname{div}\left(\frac{1}{T} \left(\rho u \vec{v} + \mu_{d} + D_{d} + \vec{\nabla} C_{d} + \mu_{t} + D_{t} + \vec{\nabla} C_{t} + \mu_{p} + D_{p} + \vec{\nabla} C_{p} + \mu_{t} + D_{t} + \vec{\nabla} C_{t} + \mu_{p} + D_{p} + \vec{\nabla} C_{p} + \mu_{t} + \mu_{t} + D_{t} + \vec{\nabla} C_{t} + \mu_{t} + \mu_{t} + D_{t} + \vec{\nabla} C_{t} + \mu_{t} + \mu_{p} + D_{p} + \vec{\nabla} C_{p} + \vec{\nabla} C_{p} + \mu_{t} + \mu_{t$$

In this formula  $E_i$ , i = 1, 2, 3, are measured in joules. The total free energy production is given by the formula

$$\widetilde{F} = \iiint_V \frac{df}{dt} \, dv \tag{85}$$

where all quantities are solutions of variational problem.

Using some results from our investigations, especially T = const, one gets for  $\frac{df}{dt}$ 

$$\frac{df}{dt} = \frac{1}{\rho} \left( \operatorname{div}(\rho u \vec{v}) + \operatorname{div} \left( \mu_{d} + D_{d} + \vec{\nabla} C_{d} + \mu_{t} + D_{t} + \vec{\nabla} C_{t} + \mu_{p} + D_{p} + \vec{\nabla} C_{p} + \mu_{3} + \mu_{3} + \mu_{n} \nabla C_{3} + \mu_{n} D_{n} \vec{\nabla} C_{n} + \mu_{4} + \mu_{e} D_{4} + \mu_{e} \nabla C_{4} + \mu_{e} + \mu_{\gamma} D_{\gamma} \vec{\nabla} C_{\gamma} \right) 
- \left( D_{d} + \vec{\nabla} C_{d} + \vec{\nabla} \mu_{d} + D_{t} + \vec{\nabla} C_{t} + \vec{\nabla} \mu_{t} + D_{p} + \vec{\nabla} C_{p} + \vec{\nabla} \mu_{p} + \mu_{e} + D_{3} + \vec{\nabla} C_{3} + \vec{\nabla} \mu_{3} + D_{n} \vec{\nabla} C_{n} \vec{\nabla} \mu_{n} + D_{4} + \vec{\nabla} C_{4} + \vec{\nabla} \mu_{4} + D_{\gamma} \vec{\nabla} C_{\gamma} \vec{\nabla} \mu_{\gamma} \right) 
- \frac{\varphi \rho_{H} B_{F} \lambda_{(dF)} \lambda_{(dFd)} + (B_{1} (\mu_{t} + M_{t} + \mu_{p} + M_{p} +$$

Let us denote by  $V \subset \mathbb{R}^3$  a set of a shape of a sample and by  $\partial V$  its boundary. Let us notice that V means also a volume of a sample. Moreover, it does not result in any misunderstanding. Let us define boundary conditions of our set of elliptic equations (73)–(79), (80) and (81) with (82), Eqs (83a)–(83g), i.e.

$$c_i|_{\partial V} = \widetilde{c}_i \tag{87}$$

$$\mu_i|_{\partial V} = \widetilde{\mu}_i \tag{88}$$

where the functions  $\tilde{c}_i$  and  $\tilde{\mu}_i$  are defined on  $\partial V$ . One also gets

$$B_{1}(\widetilde{\mu}_{t+}M_{t+} + \widetilde{\mu}_{p+}M_{p+}) + B_{2}(\widetilde{\mu}_{^{3}\text{He}}M_{^{3}\text{He}} + \widetilde{\mu}_{n}M_{n}) + B_{3}(\widetilde{\mu}_{^{4}\text{He}}M_{^{4}\text{He}} + \widetilde{\mu}_{\gamma}M_{\gamma}) = 2\widetilde{\mu}_{d+}M_{d+}.$$
(89)

Solutions of Laplace equations can be obtained via elementary analytical or numerical methods. Afterwards we should consider Eqs (73)–(79). The best way to solve these equations is to use a Green function method. The Green function for V with  $\partial V$  is defined as follows:

$$\vec{\nabla}^2 G = -\delta(x - \xi, y - \eta, z - \zeta) \tag{90}$$

if  $(x, y, z) \in V$  and G = 0 if  $(x, y, z) \in \partial V$ , where  $G(x, y, z, \xi, \eta, \zeta)$  is a function of 6 variables singular if

$$x \to \xi$$
 or  $y \to \eta$  or  $z \to \zeta$ .

The solutions for Eqs (80) are given by

$$\mu_i(\xi, \eta, \zeta) = \iint_{\partial V} \frac{\partial G}{\partial n} \, \widetilde{\mu}_i \, ds \tag{91}$$

where  $\frac{\partial G}{\partial n}$  is the normal derivative of G on  $\partial V$ .

For Eq. (81) one gets

$$C_i(\xi, \eta, \zeta) = \kappa K_i \iiint_V G \, dv + \iiint_{\partial V} \frac{\partial G}{\partial n} \, \widetilde{c}_i \, ds. \tag{92}$$

Moreover, we need  $C_i$  also as a function of  $\varphi$ 

$$C_{i}(\varphi, \xi, \eta, \zeta) = \varphi \widetilde{K}_{i} \iiint_{V} G \, dv + \iiint_{\partial V} \frac{\partial G}{\partial n} \, \widetilde{c}_{i} \, ds, \tag{93}$$

where

$$\widetilde{K}_i = \frac{B_F \rho_H \lambda_{(dF)} \lambda_{(dFd)^+}}{N_A} K_i. \tag{94}$$

We solve Eqs (73)–(79) for various values of  $\varphi$  and put all the solutions to Eq. (55) in order to get equations for

$$\rho u\vec{v} = \vec{w} \tag{95}$$

$$\operatorname{div} \vec{w} = \widetilde{f}(\vec{r})$$

$$\vec{r} = (x, y, z) \in V \subset \mathbb{R}^3$$
(96)

One easily gets

$$\widetilde{f}(\vec{r}) = -\varphi \left[ \frac{D_{d^{+}} \widetilde{K}_{d^{+}}}{2M_{d^{+}}} \iint_{\partial V} ds \, \frac{\partial G}{\partial n} \left( B_{1} \left( \widetilde{\mu}_{t^{+}} M_{t^{+}} + \widetilde{\mu}_{p^{+}} M_{p^{+}} \right) + B_{2} \left( \widetilde{\mu}_{{}^{3}\text{He}} M_{{}^{3}\text{He}} + \widetilde{\mu}_{n} M_{n} \right) \right. \\
+ B_{3} \left( \widetilde{\mu}_{{}^{4}\text{He}} M_{{}^{4}\text{He}} + \widetilde{\mu}_{\gamma} M_{\gamma} \right) \right) + D_{p^{+}} \widetilde{K}_{p^{+}} \iint_{\partial V} ds \, \frac{\partial G}{\partial n} \, \widetilde{\mu}_{p^{+}} \\
+ D_{{}^{3}\text{He}} \widetilde{K}_{{}^{3}\text{He}} \iint_{\partial V} ds \, \frac{\partial G}{\partial n} \, \widetilde{\mu}_{{}^{3}\text{He}} + D_{n} \widetilde{K}_{n} \iint_{\partial V} ds \, \frac{\partial G}{\partial n} \, \widetilde{\mu}_{n} + D_{t^{+}} \widetilde{K}_{t^{+}} \iint_{\partial V} ds \, \frac{\partial G}{\partial n} \, \widetilde{\mu}_{t^{+}} \\
+ D_{{}^{4}\text{He}} \widetilde{K}_{{}^{4}\text{He}} \iint_{\partial V} ds \, \frac{\partial G}{\partial n} \, \widetilde{\mu}_{{}^{4}\text{He}} + D_{\gamma} \widetilde{K}_{\gamma} \iint_{\partial V} ds \, \frac{\partial G}{\partial n} \, \widetilde{\mu}_{\gamma} \right] \quad (97)$$

We suppose a potential flow

$$\vec{v} = \vec{\nabla}R,\tag{98}$$

where R is a velocity potential.

Thus one gets

$$\operatorname{div}(\rho u \vec{\nabla} R) = \widetilde{f}(\vec{r}). \tag{99}$$

Simultaneously we have a continuity equation

$$\operatorname{div}(\rho \vec{v}) = 0 \tag{100}$$

or 
$$\operatorname{div}(\rho \vec{\nabla} R) = 0.$$
 (101)

Supposing equation

$$u = u(T, \rho) \tag{102}$$

one eventually gets

$$\begin{cases}
\rho \frac{\partial u}{\partial \rho} \vec{\nabla} \rho \vec{\nabla} R = \widetilde{f}(\vec{r}) \\
\vec{\nabla} \rho \vec{\nabla} R + \vec{\nabla}^2 R = 0.
\end{cases}$$
(103)

We can solve system Eqs (103) under boundary conditions

$$R|_{\partial V} = \widetilde{R}, \quad \rho|_{\partial V} = \widetilde{\rho}$$

where  $\widetilde{R}$  and  $\widetilde{\rho}$  are functions defined on  $\partial V$ . Afterwards we put solutions and Eq. (103) to Eq. (86) with several values of  $\varphi$  getting from Eq. (85) a total free energy production,  $\widetilde{F}$ . We suppose

$$p = p(T, \rho). \tag{104}$$

From Eq. (86) one easily gets

$$\frac{df}{dt} = -\frac{p}{\rho} \vec{\nabla}^2 R + \frac{1}{N_A} \varphi \lambda_{(dF)} \lambda_{(dFd)} + B_F \rho_H (B_1 E_1 + B_2 E_2 + E_3). \tag{105}$$

Eqs (85), (102), (103), (104), (105) give us a simple theory of our cold fusion reactor (together with all boundary conditions). The system of Eqs (103) forms a nonlinear system of pde. In this way even if it is elliptic we can expect some interesting phenomena for  $\widetilde{F}$  connecting to soliton-like solutions. This demands more investigations and will be done elsewhere.

Functions u and p depend on the material of a sample and can be obtained from physico-chemical tables.

Let us notice that we can consider also a bound system of deuteron–deuteron–quasiparticle in such a case where a charge quasiparticle is screening a Coulomb barrier. In this way a tunnel effect has higher probability. The mentioned quasiparticle could have a different statistics than Fermi–Dirac statistics, i.e. Böse–Einstein statistics. This situation is similar to  $\pi^-$ -atoms and  $\pi^-$ -molecules. (We should prevent  $\pi$ -meson to interact strongly with nuclei.) One can also try to design 2-dimensional systems interacting with deuterons. In this case we can have to do with anyons as the third particle in three-bodies interacting bound system. The important point is to find such materials where such charged quasiparticles are heavy and their states are narrow. They should screen the Coulomb barriers to make a tunnel effect more probable.

There is also a possibility to employ negatively charged solitons known in solid state physics in order to lower a Coulomb barrier in a three bodies interactions (i.e. deuteron–deuteron–soliton). In superconducting materials such solitons are possible to exist. In calculation of binding energy of such quasimolecules we can follow e.g. Ref. [18].

Recently there is an interest in some exotic molecules with some different particles than electrons and nuclei. It means molecules with  $\mu^+$  particles in place of protons and also with positrons  $e^+$  except very well known mesoatoms (see Refs [19], [20]). Our approach to nuclear fusion is based on similar ideas. Moreover, we consider molecules with quasiparticles in solid state physics coupled to ordinary nuclei.

More advanced quantum chemistry treatment of exotic molecules appropriate for further studies can be found in Ref. [21].

Low Energy Nuclear Reactions (LENR) sometimes called Chemically Assisted Nuclear Reactions are still under investigations all around the world (see Refs [22, 23, 24, 25, 26, 27]).

An effective interaction between hydrogen atoms (deuterium atoms) in a solid can be intuitively described as quasichemical bonds in quasimolecules. These quasimolecules involve quasiparticles and ordinary particles. In particular, heavy fermions in solids and hydrogen or deuterium nuclei. Such an approach is similar to muon catalysis in cold fusion and we can use some intuition from the approach. The heavy fermion catalysis paradigm can help us to find some materials where such a cold fusion is very probable and to check them for further investigations. This is the aim of the paper.

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