

Theory of Low-Energy Deuterium Fusion in Micro/Nano-Scale Metal Grains and Particles

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Abstract

A consistent conventional theoretical description is presented for anomalous low-energy deuterium nuclear fusion in micro/nano-scale metal grains and particles. The theory is based on the Bose-Einstein condensate (BEC) state occupied by deuterons trapped in a micro/nano-scale metal grain or particle. The theory is capable of explaining most of the experimentally observed results and also provides theoretical predictions. Experimental tests of theoretical predictions are proposed. Scalabilities of the observed effects are discussed based on theoretical predictions.

1. Introduction

The conventional deuterium fusion in free space proceeds via the following nuclear reactions:

- {1} $D+D \rightarrow p(3.02 \text{ MeV}) + T(1.01 \text{ MeV})$;
- {2} $D+D \rightarrow n(2.45 \text{ MeV}) + {}^3\text{He}(0.82 \text{ MeV})$; and
- {3} $D+D \rightarrow {}^4\text{He} + \gamma(23.8 \text{ MeV})$.

The cross-sections (or reaction rates) for reactions {1} – {3} have been measured by beam experiments at intermediate energies ($\geq 10 \text{ keV}$), and are expected to be extremely small at low energies ($\leq 10 \text{ eV}$) due to the Gamow factor arising from Coulomb barrier between two deuterons. The measured cross-sections have branching ratios: $(\sigma\{1\}, \sigma\{2\}, \sigma\{3\}) \approx (1, 1, 10^{-6})$.

From many experimental measurements by Fleischmann and Pons in 1989, and many others over 19 years since then [1], including the recent work by Szpak, Mosier-Boss, and Gordon [2] and the most recent work by Arata and Zhang [3], the following fact has been established. At ambient temperatures or low energies ($\leq 10 \text{ eV}$), deuterium fusion in metal proceeds via the following reactions:

- {4} $D(m) + D(m) \rightarrow p(m) + T(m) + 4.03 \text{ MeV} (m)$;
- {5} $D(m) + D(m) \rightarrow n(m) + {}^3\text{He}(m) + 3.27 \text{ MeV} (m)$; and
- {6} $D(m) + D(m) \rightarrow {}^4\text{He}(m) + 23.8 \text{ MeV} (m)$,

where m represents a host metal lattice or metal particle. Reaction rate R for {6} is dominant over reaction rates for {4} and {5}, i.e., $R\{6\} \gg R\{4\}$ and $R\{6\} \gg R\{5\}$. Additional experimental observations include requirements of both higher deuteron loading ($D/Pd \geq 1$) and deuterium purity ($H/D \ll 1$), the phenomenon of “heat after death”, and enhancement of the

effect by electromagnetic fields and laser stimulation. In this paper, a consistent conventional theoretical description is presented for explaining the above observations of deuterium nuclear fusion in micro/nano-scale metal grains and particles. The theory presented in this paper is capable of explaining the above observations, and provides theoretical predictions which can be tested experimentally for the confirmation of the theory.

In the following, a detailed description of the theoretical explanation, based on the theory of Bose-Einstein condensation nuclear fusion (BECNF) [4-7] and on selection rules recently derived for a mixed system of two species [8], will be presented along with suggested experimental tests of predictions of the theory and a discussion of the scalability of the fusion rates based on the theory.

2. Theory of Bose-Einstein Condensation Nuclear Fusion (BECNF)

Bose-Einstein condensation (BEC) mechanism: The concept of the Bose-Einstein condensation (BEC) [9] has been known for 84 years (since 1924), and has been used to describe all physical scales, including liquid ^4He , excitons in semiconductors, pions and kaons in dense nuclear matter (neutron stars, supernovae), and elementary particles [10]. It is only 13 years ago in 1995 that the BEC phenomenon was observed directly in dilute vapors of alkali atoms, such as rubidium [11], lithium [12], and sodium [13] confined in magnetic traps and cooled down to nano Kelvin temperatures.

In the atomic BEC case [11], the BEC state was created by cooling dilute Rb atoms loaded into a magnetic confinement potential at 300 K. It was cooled by laser cooling (Doppler cooling) to $\sim 90 \mu\text{K}$ (4×10^6 atoms) with a density of 2×10^{10} atoms/cm³. Further cooling was accomplished by evaporation cooling removing energetic atoms to 170 nK. At 170nK, it consists of 2000 atoms at a number density of 2.6×10^{12} /cm³ in BEC state (near zero velocity) while other 2×10^4 atoms in the trap had a Maxwell-Boltzmann (MB) velocity distribution with an exponential tail characteristic of $T \approx 170\text{nK}$. The requirement for BEC, $\lambda_{\text{db}} > d$, is satisfied, where λ_{db} is the de Broglie wavelength and d is interatomic spacing distance.

In our nuclear BEC phenomenon, we have deuteron number density of $\sim 6.8 \times 10^{22}$ cm⁻³ in metal, corresponding to an average separation distance of $d \approx 2.45 \text{ \AA}$ between deuterons. In order to achieve the nuclear BEC state of deuterons in metal, we need to have the average deuteron kinetic energy T_d smaller than $T_d^c = 0.0063 \text{ eV}$, i.e. $T_d < T_d^c$, in order to satisfy the requirement $\lambda_{\text{db}} > d$.

The MB distribution is originally derived for weakly interacting dilute gas (ideal gas). For strongly interacting and dense systems such as mobile deuterons in metal, the MB distribution is not applicable and hence average deuteron kinetic energy of $kT = 0.026 \text{ eV}$ at $T = 300 \text{ K}$ is not applicable for deuterons in metal.

Mobility of deuterons in a metal is a complex phenomenon and may involve a number of different processes [14]: coherent tunneling, incoherent hopping, phonon-assisted processes, thermally activated tunneling, and over-barrier jump/fluid like motion at higher temperatures. If mobile deuterons in a metal are confined by a confining potential provided by metal atoms and electrons, it may be possible that deuteron momentum or velocity distribution in a metal may have the average deuteron kinetic energy smaller than $T_d^c = 0.0063 \text{ eV}$, thus satisfying $\lambda_{\text{db}} > d$.

We note that $T_d^c = 0.0063 \text{ eV}$ corresponds to the average deuteron velocity of $v_c = 0.78 \times 10^5$

cm/sec while the average deuteron kinetic energy of $kT = 0.026$ eV with $T = 300$ K corresponds to the average deuteron velocity of $v_k = 1.6 \times 10^5$ cm/sec. Boundaries for micro/nano-scale metal grains and particles can act as barriers and may slow down mobile deuterons resulting in lower average velocity $v < v_c$ and smaller average kinetic energy $T_d < T_d^c$ near boundaries. Therefore, it may be possible that the conditions, $T_d < T_d^c$ and $\lambda_{db} > d$, are achieved for mobile deuterons in localized regions of the metal without cooling as done in the atomic BEC case, and hence, it may be possible to observe experimentally the effects of the nuclear BEC.

Mobility of proton and deuteron in metals: It is well known that the hydrogen ions are highly mobile within metal hydrides [14,15]. Hydrogen mobility takes various temperature dependent forms. The mobility extends to “fluid like” motion at temperatures comparable to the interstitial site or self-trapping, binding energy ~ 0.15 eV. At higher temperatures below the melting point, hydrogen ions no longer remain within the potential wells of interstitial sites but undergo free motion similar to the motion of atoms in gases [14]. It is expected that the mobility of hydrogen ions (or deuterium ions) will increase, as the loading ratio H/metal (or D/metal) of hydrogen atoms (or deuterium atoms) increases and becomes larger than one, $H/metal \geq 1$ (or $D/metal \geq 1$).

Theoretical formulation for single species case: For applying the concept of the BEC mechanism to deuterium fusion in a nano-scale metal particle, we consider N identical charged Bose nuclei (deuterons) confined in an ion trap (or a metal grain or particle). Some fraction of trapped deuterons are assumed to be mobile as discussed above. For simplicity, we assume an isotropic harmonic potential for the ion trap to obtain order of magnitude estimates of fusion reaction rates. N -body Schrodinger equation for the system is given by

$$H\Psi = E\Psi \quad (1)$$

with the Hamiltonian H for the system given by

$$H = \frac{\hbar^2}{2m} \sum_{i=1}^N \Delta_i + \frac{1}{2} m\omega^2 \sum_{i=1}^N r_i^2 + \sum_{i<j} \frac{e^2}{|r_i - r_j|} \quad (2)$$

where m is the rest mass of the nucleus. The detailed derivations are given elsewhere [5,6,7,16] for obtaining the approximate the ground state solution for Eq. (1) and the approximate theoretical formula for the deuteron-deuteron fusion rate in an ion trap (nano-scale metal particle). The use of an alternative method based on the mean-field theory for bosons (see Appendix in [6]) yields the same result.

Our final theoretical formula for the nuclear fusion rate R_{trap} for a single trap containing N deuterons is given by

$$R_{\text{trap}} = \Omega B N \omega^2 \quad (3)$$

$$\text{with } \omega^2 = \sqrt{\frac{3}{4\pi}} \alpha \left(\frac{\hbar c}{m} \right) \frac{N}{\langle r \rangle^3} \quad (4)$$

where $\langle r \rangle$ is the radius of trap/atomic cluster, $\langle r \rangle = \langle \Psi | r | \Psi \rangle$, N is the average number of Bose nuclei in a trap/cluster, and B is given by $B = 3 A m / (8\pi \alpha \hbar c)$, with $A = 2 S r_B / (\pi \hbar)$, $r_B = \hbar^2 / (2\mu e^2)$, and $\mu = m/2$. S is the S -factor for the nuclear fusion reaction between two deuterons. For $D(d,p)T$ and $D(d,n)^3\text{He}$ reactions, we have $S \approx 55$ keV-barn. We expect also $S \approx 55$ keV-barn for reaction $\{6\}$.

Only one unknown parameter is the probability of the BEC ground state occupation, Ω . It may be proportional to $N^{-1/3}$, $\Omega \propto N^{-1/3}$, or to N^{-2} , $\Omega \propto N^{-2}$.

We can rewrite Eq. (3) as

$$R_{\text{trap}} = 4(3/4\pi)^{3/2} \Omega A \frac{N^2}{D_{\text{trap}}^3} \propto \Omega \frac{N^2}{D_{\text{trap}}^3} \quad (5)$$

where D_{trap} is the average diameter of the trap, $D_{\text{trap}} = 2\langle r \rangle$.

The total fusion rate R_t is given by

$$R_t = N_{\text{trap}} R_{\text{trap}} = \frac{N_D}{N} R_{\text{trap}} \propto \Omega \frac{N}{D_{\text{trap}}^3} \quad (6)$$

where N_D is the total number of deuterons and $N_{\text{trap}} = N_D/N$ is the total number of traps.

Two species case and selection rule: We consider a mixture of two different species of positively charged nuclear particles, labeled 1 and 2, with N_1 and N_2 particles, respectively, both trapped in a micro/nano-scale metal grain or particle. We denote charges and masses as $Z_1 \geq 0$, $Z_2 \geq 0$, and m_1 , m_2 , respectively. We use the mean-field theory [7,17] for a system of interacting bosons confined in a harmonic potential to derive the following selection rule:

$$\frac{Z_1}{m_1} = \frac{Z_2}{m_2} \quad (7)$$

The detailed derivations are given in reference [8]. We now apply the selection rule, Eq. (7). If we use m as mass number approximately given in units of the nucleon mass, we have $[Z_1(\text{D})/m_1(\text{D})] = 1/2$, $[Z_2(\text{p})/m_2(\text{p})] = 1$, $[Z_2(\text{T})/m_2(\text{T})] = 1/3$, $[Z_2(\text{n})/m_2(\text{n})] = 0$, and $[Z_2(^3\text{He})/m_2(^3\text{He})] = 2/3$.

Since $[Z_1/m_1] \neq [Z_2/m_2]$ for reactions {4} and {5} they are forbidden or suppressed, and fusion reaction rates for reactions {4 and {5} are expected to be small, while reaction {6} is allowed since $[Z_1/m_1] = [Z_2/m_2]$, and fusion reaction rate is expected to be large for reaction {6}. In summary, we obtain $R\{6\} \gg R\{4\}$ and $R\{6\} \gg R\{5\}$.

3. Theoretical Implications and Predictions

Eqs. (3) and (6) provide an important result that nuclear fusion rates R_{trap} and R_t do not depend on the Gamow factor in contrast to the conventional theory for nuclear fusion in free space. This could provide explanations for overcoming the Coulomb barrier and for the claimed anomalous effects for low-energy nuclear reactions in metals.

This is consistent with the conjecture noted by Dirac [18] and used by Bogolubov [19] that boson creation and annihilation operators can be treated simply as numbers when the ground state occupation number is large. This implies that for large N each charged boson behaves as an independent particle in a common average background potential and the Coulomb interaction between two charged bosons is suppressed.

For a single trap (or metal particle) containing N deuterons, the deuteron-deuteron fusion can proceed with the following three reaction channels.

$$\begin{aligned}
\psi_{BEC} \{ (N-2)D's + (D+D) \} &\rightarrow \psi^* \{ {}^4\text{He} + (N-2)D's \} \quad (Q = 23.84 \text{ MeV}) \\
&\psi^* \{ T + p + (N-2)D's \} \quad (Q = 4.03 \text{ MeV}) \\
&\psi^* \{ {}^3\text{He} + n + (N-2)D's \} \quad (Q = 3.27 \text{ MeV})
\end{aligned}$$

where ψ_{BEC} is the Bose-Einstein condensate ground state (a coherent quantum state) with N deuterons and ψ^* are final excited continuum states. Excess energy (Q value) is absorbed by the BEC state and shared by (N-2) deuterons and reaction products in the final state.

We now consider the total momentum conservation. The initial total momentum of the initial BEC state with N deuterons (denoted as D^N) is given by $\bar{P}_{D^N} \approx 0$. Because of the total momentum conservation, the final total momenta for reactions {4}, {5}, and {6} are given by

$$\begin{aligned}
\{4\} \quad \bar{P}_{D^{N-2}pT} &\approx 0, \quad \langle T_D \rangle \approx \langle T_p \rangle \approx \langle T_T \rangle \approx Q\{4\}/N \\
\{5\} \quad \bar{P}_{D^{N-2}n{}^3\text{He}} &\approx 0, \quad \langle T_D \rangle \approx \langle T_n \rangle \approx \langle T_{{}^3\text{He}} \rangle \approx Q\{5\}/N \\
\{6\} \quad \bar{P}_{D^{N-2}{}^4\text{He}} &\approx 0, \quad \langle T_D \rangle \approx \langle T_{{}^4\text{He}} \rangle \approx Q\{6\}/N
\end{aligned}$$

where T represents the kinetic energy.

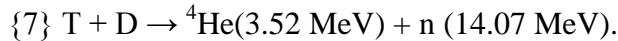
For a micro-scale metal grain confined by grain boundaries of $\sim 1\mu\text{m}$ diameter, we expect to have $N \approx 10^{10}$ and $Q\{6\}/N \approx 10^{-3} \sim 10^{-4}$ eV, and hence we expect the excess heat and ${}^4\text{He}$ production due to reaction {6} but no nuclear ashes from some of the reactions described below in section 4.

For nano-scale metal particles, the above consideration shows that excess energies (Q) lead to a micro/nano-scale fire-work type explosion, creating a crater/cavity and a hot spot with fire-work like star tracks. The size of a crater/cavity will depend on number of neighboring Pd nanoparticles participating in BEC fusion almost simultaneously. Since sizes of deuteron and Pd nucleus are of the order of $\sim 10^{-4} \text{ \AA}$ (~ 10 fm) while the average distance between two neighboring Pd atoms is $\sim 2.5 \text{ \AA}$, ~ 10 keV deuteron from the BEC deuterium fusion encounters mostly electrons and transfers its kinetic energy to electrons. Occasionally, ~ 10 keV deuteron may interact with Pd nucleus to initiate nuclear reactions, Pd(d,p)Rh, etc. When the BEC deuterium fusion takes place in a Pd nanoparticle, exploding deuterons are expected to damage and leave the host Pd nanoparticle, but some of the Pd nanoparticles may remain intact and may participate again in the BEC deuterium fusion after absorbing again a sufficient number of deuterons, $D/Pd \geq 1$.

4. Further Consequences of BEC Mechanism and of Selection Rule

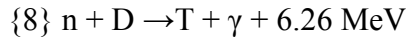
Effects due to deuterons: Deuterons with $Q\{6\}/N \approx \sim 10$ keV energy from reaction {6} can undergo reactions {1} and {2} producing p(3.02 MeV), T(1.01 MeV), n(2.45 MeV), and ${}^3\text{He}$ (0.82 MeV), which in turn will proceed with further reactions.

Tritons produced by reaction {1} (1.01 MeV triton) and by reaction {4} (average kinetic energy of $Q\{4\}/N \approx \sim \text{keV}$) will interact with surrounding deuterons via the following reaction



Because of triton kinetic energies of 1.01 MeV or \sim keV, the reaction rate for {7} could be large enough to produce 14.07 MeV neutrons, which may have been recently observed by Forsley and Mosier-Boss [20]. We note that ^4He produced by reaction {7} has much higher kinetic energy (3.52 MeV) compared with deuterons from reaction {6} ($Q\{6\}/N \approx \sim 10$ keV).

Effects due to neutrons: Neutrons with 2.45 MeV kinetic energy from reaction {2}, neutrons with $Q\{5\}/N \approx \sim$ keV kinetic energy from reaction {5}, or neutrons with 14.07 MeV kinetic energy from reaction {7} can undergo further reactions, {8} and/or {9} below:



{9} Neutron induced transmutation with other nuclei.

In addition, 14.07 MeV neutrons from reaction {7} may initiate reactions, $^{12}\text{C}(n,n')^3\text{He}$ and $^{12}\text{C}(n,n')^8\text{Be} (^8\text{Be} \rightarrow 2^4\text{He})$, which may have been recently observed by Mosier-Boss et al. [21].

Since reaction {8} produces more tritiums than neutrons, we expect $R(\text{T}) > R(\text{n})$, and also $R(\text{T}) > R(^3\text{He})$.

High deuterium loading requirement: $\text{D}/\text{Pd} \geq 1$ is required for sustaining deuteron mobility in Pd metal. The mobility of deuterons is required for the BEC mechanism.

Deuterium purity requirement: Because of violation of the selection rule, $[Z_1(\text{D})/m_1(\text{D})] \neq [Z_2(\text{p})/m_2(\text{p})]$, presence of hydrogens in deuteriums will suppress the formation of the BEC states, thus diminishing the fusion rate due to the BEC mechanism. The required H/D ratio is expected to be $\text{H}/\text{D} < N^{-1}$. For a 5 nm Pd nanoparticle with $N \approx 10^4$, $\text{H}/\text{D} < 10^{-4}$, and hence 99.99 % deuterium purity is required.

Heat after death: There have been observations of continued heat generation after the input for experiment is switched off. This effect is known as “heat after death”. Because of mobility of deuterons in Pd particle traps, a system of $\sim 10^{22}$ deuterons contained in $\sim 10^{18}$ Pd particle traps (in 3g of Pd particles with average particle diameter of $\sim 50 \text{ \AA}$) is a dynamical system. BEC states are continuously attained in a small fraction of the $\sim 10^{18}$ Pd particle traps and undergo BEC fusion processes, until the formation of the BEC state ceases or becomes negligible.

Enhancement by electromagnetic fields and laser stimulation: Application of electromagnetic fields [2] and laser stimulation [22] have been shown to enhance the excess heat production and other anomalous effects. These effects may be due to a decrease of the average kinetic energy of mobile deuterons and/or to an increase of mobile deuterons participating in the BEC fusion processes.

Increase of resistance: When the BECNF occurs, more mobile deuterons will be created. This in turn will increase the resistance of metal. This effect may have been recently observed by Celani et al. in deuterium gas loading experiments with Pd nanoparticles coated on a Pd wire [23].

5. Experimental Tests of Theoretical Predictions

The first experimental test of the BEC mechanism for deuterium fusion with nano-scale Pd particles was carried out with Pd blacks loaded by high-pressure deuterium gas [16]. The result of this experiment shows no excess heat production. This may be due to the fact that Pd nanoparticles (Pd Blacks) used had too large sizes (80 nm – 180 nm) and were clumped together

(not isolated). Furthermore, deuterium purity requirement was not satisfied. The recent report of deuteron gas-loading experiment by Arata and Zhang [3] show positive results of observing excess heat and ^4He production using ~ 5 nm Pd particles imbedded in ZrO_2 and purified deuterium. For experimental tests of the predictions of the theory, it would be advantageous scientifically to use samples of Pd nanoparticles deposited on thin films such as $\text{Al}_2\text{O}_3/\text{NiAl}(111)$ [24-26], even though bulk materials such as Pd nanoparticles imbedded in SiO_2 aerogels [27] are more suitable for practical applications. Other possibilities are to use other metals such as Zr or Ti nanoparticles. In all cases, the theory requires that metal nanoparticles and micrograins are to be separated from each other by boundaries.

Tests based on the average size of metal particles: From Eq. (6) with $N=N_D(\pi/6)D_{\text{trap}}^3$, we obtain $R_t(D_{\text{trap}}) \propto D_{\text{trap}}^{-1}$ or D_{trap}^{-6} , where D_{trap} is the average trap diameter, assuming $\Omega \propto N^{-1/3}$ or N^{-2} , respectively. This can be tested experimentally. This result provides a theoretical justification for using 50 Å Pd nanoparticles to maximize the total fusion rates.

Tests based on the temperature dependence: Since the probability Ω of the BEC ground state occupation increases at lower temperatures ($\Omega \approx 1$ near $T \approx 0$), the total fusion rate R_t will increase at lower temperatures, $R_t(T_{\text{low}}) > R_t(T_{\text{high}})$. However, R_t is proportional to N_D where N_D is the total number of mobile deuterons. Since $N_D(T_{\text{low}}) < N_D(T_{\text{high}})$, we expect $R_t[N_D(T_{\text{low}})] < R_t[N_D(T_{\text{high}})]$. The above opposite temperature dependences for R_t will complicate analysis of the temperature dependence of R_t .

Tests for reaction products and heat after death: Some examples of this type of tests are (1) to look for micro/nano-scale craters/cavities and hot spots with micro/nano-scale fire-work like star tracks at Pd nanoparticle sites, before and after death, and (2) to measure neutron energies to check the reaction products carries kinetic energies of 2.45 MeV from the secondary reaction {2}, and $Q\{5\}/N \approx \sim \text{keV}$ from reaction {5}.

Tests for increase of resistance: Resistance of the metal should be measured to test predicted increase of resistance during the BECNF process.

Tests for scalability: One example is a scalability test based on the total number of N_{traps} . Since we have $R_t \propto N_{\text{trap}} R_{\text{trap}} \propto N_{\text{trap}}$ for the same R_{trap} , we have theoretical prediction,

$R_t(30\text{g Pd particles}) / R_t(3\text{g Pd particles}) \approx 10$, etc., which can be tested experimentally.

6. Conclusion and Summary

Theory of the BEC mechanism described in this paper provides a consistent conventional theoretical description of the results of many experimental works started by Fleischmann and Pons in 1989 and by many others since then [1], including the recent work of Szpak, Mosier-Boss, and Gordon [2] and the most recent work of Arata and Zhang [3]. Theory is based on the concept of nuclear Bose-Einstein condensate state for mobile deuterons trapped in a micro/nano-scale metal grain or particle, which acts as a confinement or trapping potential, similar to a magnetic trap used to observe the atomic BEC phenomenon with atoms in 1995 [11-13]. To validate this new concept of the nuclear BEC phenomenon, experimental tests for a set of key theoretical predictions are proposed. Scalabilities of the observed effects are also discussed.

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