D(H)-Cluster Langevin Code and Some Calculated Results

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[Abstract]

A PC code based on the quantum mechanical Langevin equation to simulate dynamic motion of deuterium (or hydrogen) cluster with three dimensional symmetry has been developed for studying very fast condensation or oscillation behavior in time-step of 0.001 as (1.0E-21 second) for overall time interval of several fs to 500 fs. Some numerical results are typically shown for two cases of condensation behavior; 1) reaching to ground state oscillations as for $D(H)_2^+$ ion molecule, dμd muonic molecule, 3D+ ionic molecule, 6D/OSC and others, and 2) making fast collapse to get in the strong/weak nuclear interaction range of d-d (or p-p) inter-nuclear distance as for 4D(H)/TSC, 6D(H)/Rhombic-dodecahedron, 8D(H)/Rhombic-dodecahedron and 20D(H)/Rhombic-triacontahedron.

Keywords: PC code, D(H)-cluster dynamics, ground state oscillation, fast collapse, 4D(H)/TSC, 6D(H)-Rhombic-dodecahedron, larger clusters, nuclear interaction, simulation of cold fusion

1. Introduction

Time dependent motion of deuterium (or protium) cluster is calculable by a computer code based on the quantum-mechanical Langevin equation [1, 2]. Especially the dynamics analyses of a three body d-e-d or p-e-p, a 5-body d-e-d-e-d or p-e-p-e-p (namely D_3^+ or H_3^+ ionic molecule) and a 8-body d-e-d-e-d-e-d-e (4D) or p-e-p-e-p-e-p-e (4H) cluster under the Platonic symmetry (TSC: tetrahedral symmetric condensate) are important to understand the underlying mechanisms of condensed matter nuclear reactions aka cold fusion [3]. The dynamic analysis is quite applicable to investigate time-dependent behavior of the three body system of d-muon-d after sticking of muon onto a d-e-d molecule. The QM Langevin method is also applicable for much larger clusters under the Platonic symmetry, such as 6D(H), 8D(H), 12D(H) and 20D(H) clusters.

We have made a generalized D(H)-Cluster Langevin Code revised from the original crude one [1, 2]. We show some typical calculations of 1) dynamic motion going to the

ground state, for systems having ground state eigen-values (namely steady molecules), 2) collapsing motion going to several-tens or smaller fm size transitory condensates which may cause very enhanced multi-body nuclear interactions by strong (for D) or weak (for H) boson exchange (namely multi-body fusion), and 3) oscillation motion of EQPET clusters with electron Cooper pair and quadruplet [1, 2].

A muonic d-μ-d system converged in 8.3 fs to its ground state with the inter-nuclear d-d distance of 790 fm (0.79 pm) after approximately 80 oscillations from the time when a muon stuck onto a d-e-d state with 138 pm d-d distance of the electronic D_2^+ molecule ground state. A 4D(H)/TSC cluster collapses to the "nuclear interaction size" (20 fm to 4 fm) in 1-4 fs depending on the adoption of different type of trapping potential functions (Vs2 or Vs1 potential, for instance), always. The Rhombic dodecahedron of 6D(2-) and the Rhombic triacontahedron 20D(8+) may collapse into the nuclear interaction size. Some other examples are also shown. A list of BASIC program of the Cluster Langevin code is given in Appendix.

2. Basic Methodology for QM-Langevin Calculation

The idea is based on the known QM electron wave-functions for d-e-d and d-e-e-d systems to form 3 dimensional volumetric symmetry to attain stable force-balance structure. These 3 dimensional symmetry systems are an elongated di-cone and 'regular' di-cone, respectively for 2D+ and D_2 molecule [2]. The ground state QM electron wave function for a d-e-d (or p-e-p) three body system is a linearly combined two 1S wave functions [2, 4], where each 1S wave function is for each D(H)-atom ground state of the d-e-d (or p-e-p) system. In Fig.1, the feature of treatment for a d-e-d system is illustrated to apply to a QM Langevin equation for calculating its dynamic motion. The ground state orbit of electron QM center is a circular rotating one with Re = Bohr radius (52.9 pm) around the mid-point of inter-nuclear d-d distance. The electron kinetic energy of d-e-d (or p-e-p) ground state is 13.6 eV that is the same value with 13.6 eV of electron kinetic energy of a D(H)-atom ground state. The inter-nuclear distance Rdd (or Rpp) of d-e-d (or p-e-p) ground state is 138 pm. The Coulombic trapping potential Vs1(1,1) of the d-e-d (or p-e-p) three body system is given in Appendix of Reference-[3] and also in Reference [5] and graphic view is shown in Fig.2. In the previous calculations [1, 2] for 4D/TSC, we have used the Vs2(1,1) potential for D_2 molecule or its approximate function Vs1(2,2) for a bosonized electron pair. In this paper, we will use Vs1(1,1) potential for every surface (regular triangle of d-d-d or p-p-p geometry) of various kind

of polyhedrons, as a unified potential component of polyhedral D(H)-cluster as 3D(H), 4D(H), 6D(H), 8D(H), 12D(H) and 20D(H) systems.

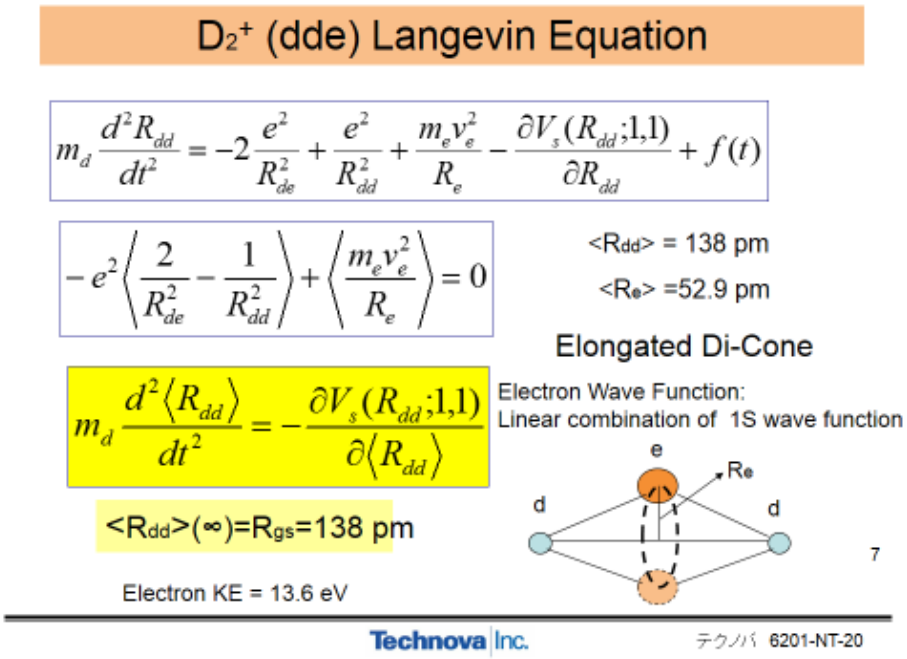

Fig.1: Treatment of dynamic motion of a d-e-d three body system by a QM Langevin equation.

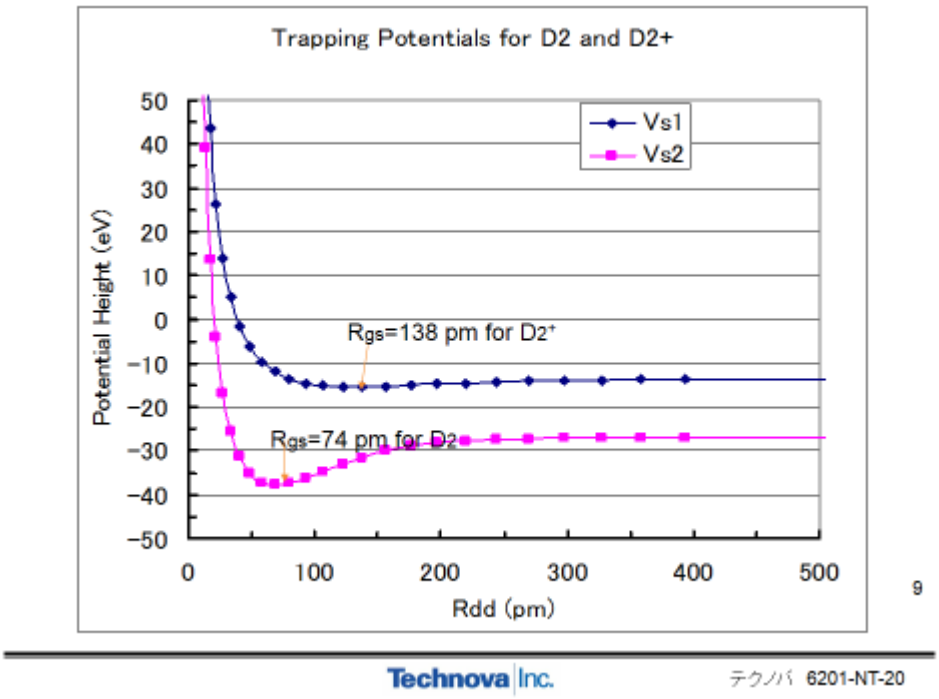

Fig.2: Coulombic trapping potential of a d-e-d system (D_2^+), compared with D_2 one.

In this paper, all mathematical equations are only described in slide-figures. Derivations of equations for the QM Langevin method are fully given in References [2, 3]. This style of paper is chosen for aiming at easier explanation of physical processes employed for making program and computations, without getting into detail of mathematics derivations.

The case of TSC is special because of double octahedral symmetry for electron wave-function and deuteron wave-function of the TS (tetrahedral symmetry) configuration. This condition makes the usage of Vs2 potential (derived from a combined 1S product-wave-functions [4, 5]) possible for the confinement force by electrons which have much larger de Broglie wave-length than deuteron wave length. In this paper, we employ a new rule for evaluating the friction term by electron QM-clouds in the QM-Langevin equation, that is the adoption of Vs1(1,1) potential always for a unit of d-d-d or p-p-p regular triangle surface configuration. We think, we have obtained similar results between the old rule (ACSLENR Vol.1 paper for 4D/TSC) and the new rule (Nf=4, Ne=6, Vs1 for 4D/TSC): the condensation time to collapse was 1.4fs and 3.6fs from 74pm to 20fm, respectively for the old and the new rule: So we may apply both rules for 4D/TSC.

When a 4D/TSC gets into the collapse region with less than about 20 fm d-d distance, strong nuclear interaction between 4 deuterons work significantly to form ^{8}Be* intermediate compound nucleus by the 4D simultaneous fusion [2, 3] and time-dependent fusion rates have been calculated using the Fermi's golden rule with estimated Coulomb barrier penetration factors (time-dependent) by the HMEQPET method [2, 3]. In the case of 4H/TSC dynamic condensation, it can get into extremely collapsed state of TSC with very small inter-nuclear p-p distances as small as Rpp=2fm, and electron capture with a proton would induce weak-strong fusion reaction to form ^{4}Li* intermediate compound state [1, 6, 7]. Nucleon halo models have been developed to study the final state interactions and ashes (nuclear products) [6, 7]. Major nuclear ashes are ^{4}He (2.0E+11 per joule) by the 4D/TSC fusion and ^{3}He and D (ca. 1.0E+12 per joule) by the 4H/TSC WS fusion, without significant hard radiations but low energy photons (BOLEP) and very weak secondary gamma-rays, respectively.

For other combinations for 3D, 6D, 8D, 12D, 20D and so forth, we do not have the double symmetry as that of 4D/TSC. (The situation is same for any H-cluster.)

So AT's idea (ACSLENRSB Vol.2 [3]) was to learn the QM electron behavior of 3D+ stable ionic molecule, for which we have experimental confirmation on 3D+ stable ion in plasma and some solutions of Schroedinger QM calculations were given [2]. The idea is to apply the confinement force of Vs1(1,1) potential for a d-e-d (or p-e-p) three body

QM system, for a basic component per a regular triangle face of total confining potential of combined D(H) polyhedral system having many faces and edges.
It is an approximate way of QM for such complicated systems as 3D+, 6D(2-), 8D(2+), 12D(8-), 20D(8+), and so on. We need careful study by cross-checking so far if the approximate approach is rational.

Because of much larger QM wave length of electrons than d(p)'s, we need a free 'rotation space' of electron QM-orbit (to satisfy HUP: Heisenberg Uncertainty Principle) for 'expectation position' for every d-d (or p-p) dipole edge. The d-e-d (2D+) system makes stable (ground state) force-balanced system as a di-cone in 3-dimensional way: the force balance holds between the central attraction force (centripetal force to the center-of-mass point) and the centrifugal force by electron rotation (circular orbit) of expectation position around the center-of-mass point (mid-point of d-d "dipole" edge). Because of **2 electrons in 3D+ system**, the circular rotation orbit can be shared for 3 d-d edges in 3-dimensional symmetric way to take balance within HUP (or electron de Broglie wave-length domain). It means, the balance is not possible in the view of classical mechanics, because only two d-d edges can share electron rotation simultaneously and the third deuteron will be kicked outside. **The HUP helps the balance for simultaneous electron sharing for 3 d-d edges and thus 3D+ can be stable quantum-mechanically.**

If we consider a 3D++ case, the regular triangle of 3d's cannot be sustained while electron is rotating around a d-d edge and therefore the third deuteron shall apart (by d-d repulsion force) from the system. Consequently, 3D++ breaks up to 2D+ (d-e-d) and deuteron. The helping force by HUP will not be enough. (We need more study here.)
Then, what will happen for 6D(2-) 3-dimensional symmetric system by 'orthogonal' combination of deuteron-octahedron and electron-cube (Rhombic Dodecahedron)?
This is our challenging problem. We think the solution by our new rule (8Nf and 12Ne) may be right. A triangle surface of deuteron-octahedron has no 'back-side' surface for an 'paired electrons' but has for an electron, so that 8 Nf will be OK as every d-d edge has sharing d-e-d type rotation orbit simultaneously to avoid break-up.
However, we are assuming that the same partial QM electron wave-function as that of the d-e-d system, namely Vs1(1,1) confining potential for a d-d pair, holds for every electron 'QM-center' on the triangle surface. The validity of this assumption shall be further studied.

For more complicated systems as 8D(2+), 12D(8-), 20D(8+), and their relative states as 'neutral' like 6D, 8D, 12D, 20D having 'fractional' net-charge of electron QM-center at a face, we do not know exactly whether the analogy of partial Vs1(1,1) friction may

hold or not.

The formulation of QM-Langevin equation for many-body polyhedral system has been derived in Reference [2]. The original form for 4D/TSC as used in Reference [3] is shown in Fig.3 with physical meaning of balance of forces between the Coulombic centripetal force, the friction by QM electron cloud and the deviation force from pure Platonic symmetry. The form of cluster trapping potential is shown accordingly.

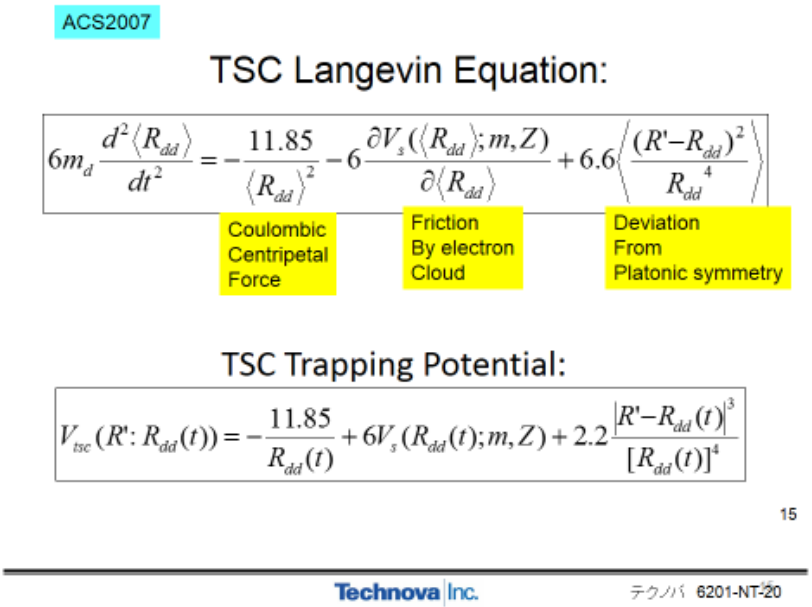

Fig.3: The QM-Langevin equation and trapping potential, originally used for Ref.[3] for 4D/TSC condensation motion.

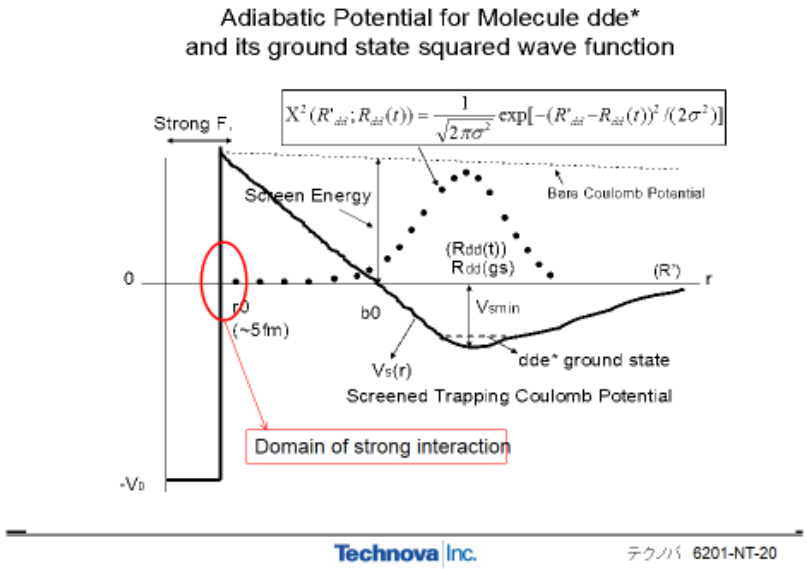

Fig.4: A d-d pair wave function, time-dependent, is approximated with Gaussian wave function

Time dependent d-d pair (for nearest d and d of polyhedron) wave function is approximated with a Gaussian wave function, adiabatically which pseudo-eigenvalue can be estimated by the HMEQPET method [2, 3]. The QM weight (barrier factor) of d-d wave function to getting into the range of strong interaction (See Fig.4) is also estimated by the WKB approximation in the HMEQPET method.

Now, our general formulas of new QM-Langevin code is shown in Fig.5 for many body polyhedral system.

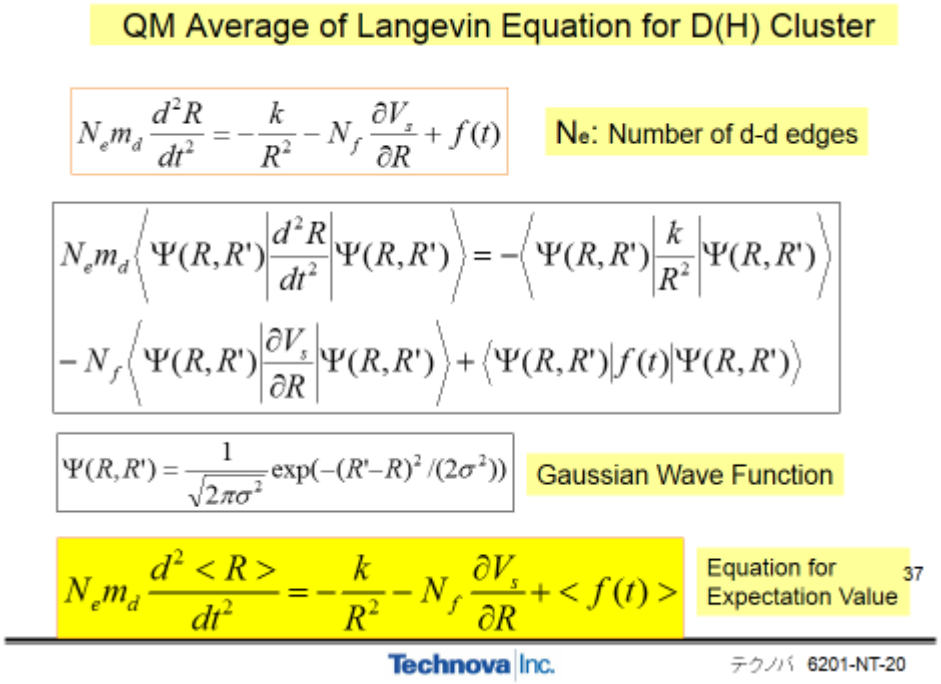

Fig.5: general formulas of QM-Langevin method for Platonic polyhedral

3. Some Calculated Results

A PC code as given in Appendix has been developed using Basic programming. We show some typical results and discussions in the following for 1) D(H)-clusters getting to stable ground state oscillations, 2) D(H)-clusters getting to collapses in nuclear strong/weak interaction ranges, and 3) virtual EQPET molecules with bosonized electrons.

3.1 **Results for Stable D(H)-Clusters**

The 3D(H)+ ionic molecule exists stably in solar plasma and accelerator ion-source plasma. The solution of the 5-body Schroedinger equation [8] has been given and

discussed in our previous paper comparing with our QM-Langevin solution, in good agreement [3]. The polyhedral structure of the 5-body d-e-d-e-d system is illustrated in Fig.6.

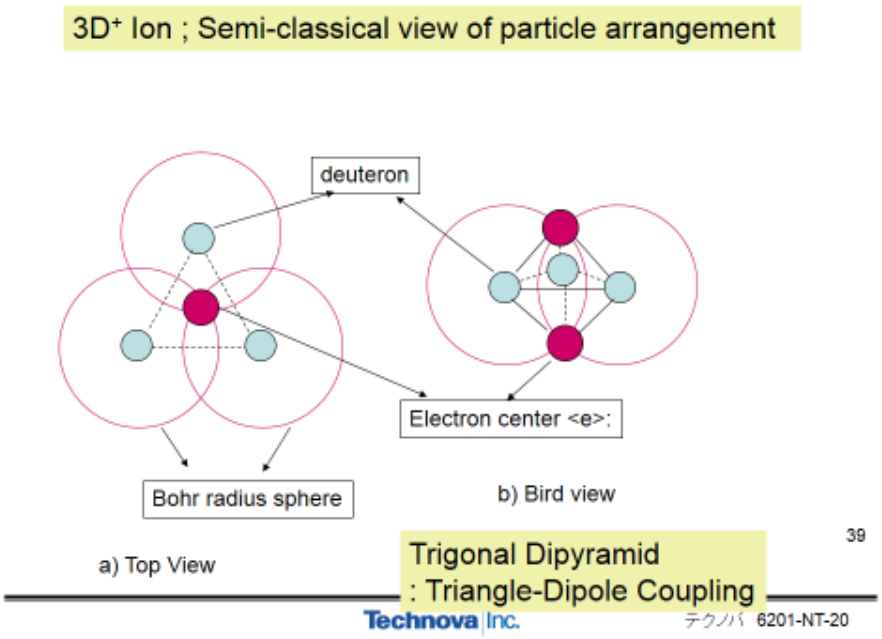

Fig.6: The polyhedral composition of 3D(H)+ ionic molecule

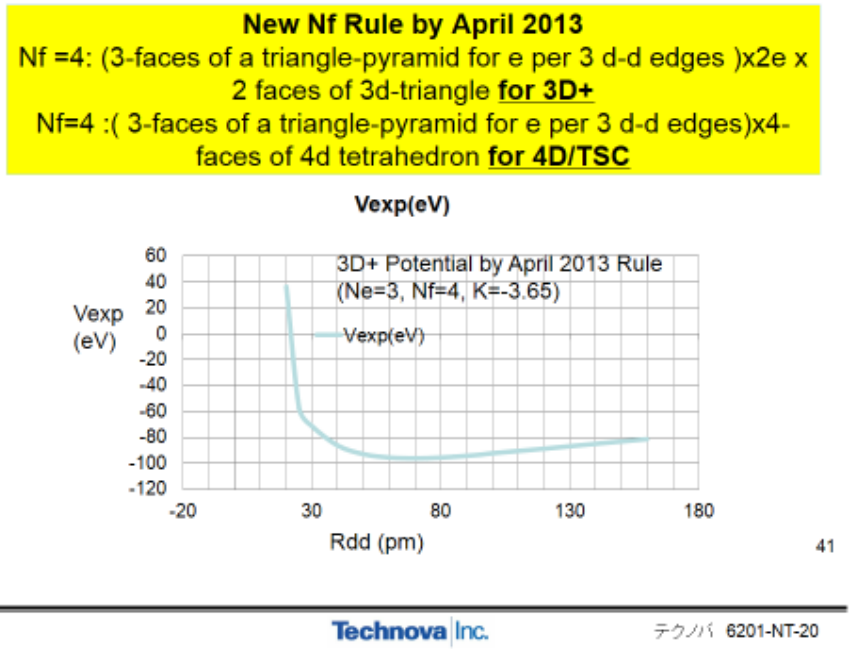

Fig.7: Trapping potential of 3D(H)+ ionic molecule, given by our new rule for QM-Langevin equation

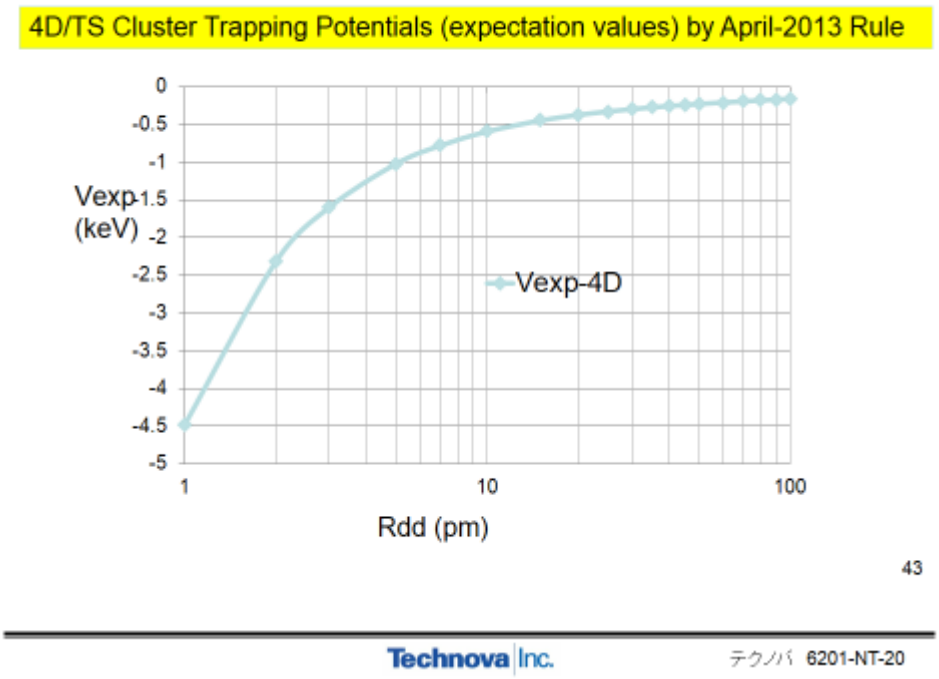

Fig.8: Trapping potential of 4D(H)/TSC by our new rule with Vs1(1,1)

Table-1: Three key parameters for QM-Langevin calculations for D(H)-clusters

Parameters for Langevin Cal.: for Electron Friction of Vs1(1,1)

Cluster	k value (keVpm)	Ne	Nf
2D+: d-e-d	0	1	1
3D+	3.65	3	4
4D/TS	11.85	6	4
6D/RD	18.45	12	8
8D/RD	18.45	12	6
12D/RT	15.51	30	20
20D/RT	19.11	30	12

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Using our new rule based on components of triangle faces with Vs1(1,1) trapping potential, the number of faces Nf =4: (3-faces of a triangle-pyramid for e per 3 d-d edges)x2e x 2 faces of 3d-triangle for 3D+ : is concluded. Its trapping potential is shown in Fig.7. The 3D(H)+ polyhedron has three d-d edges (Ne =3). Interestingly, the 4D(H)/TSC has Nf = 4 (and Ne =6) with its regular triangle surfaces, but the trapping potential shape is quite different, namely having no well-type minimum as shown in Fig.8. In Table-1, three key parameters, namely k-value of centripetal force, number of edges Ne and number of faces Nf are given for various polyhedrons. D. Rocha has calculated k-values for various configuration of polyhedral, using an excel sheet calculation by summing up all components of attractive and repulsive Coulombic potentials for possible d-d, d-e and e-e distances between QM charge centers.

The initial two oscillations of 3D+ cluster by the present D(H)-cluster Langevin code is shown in Fig.9.

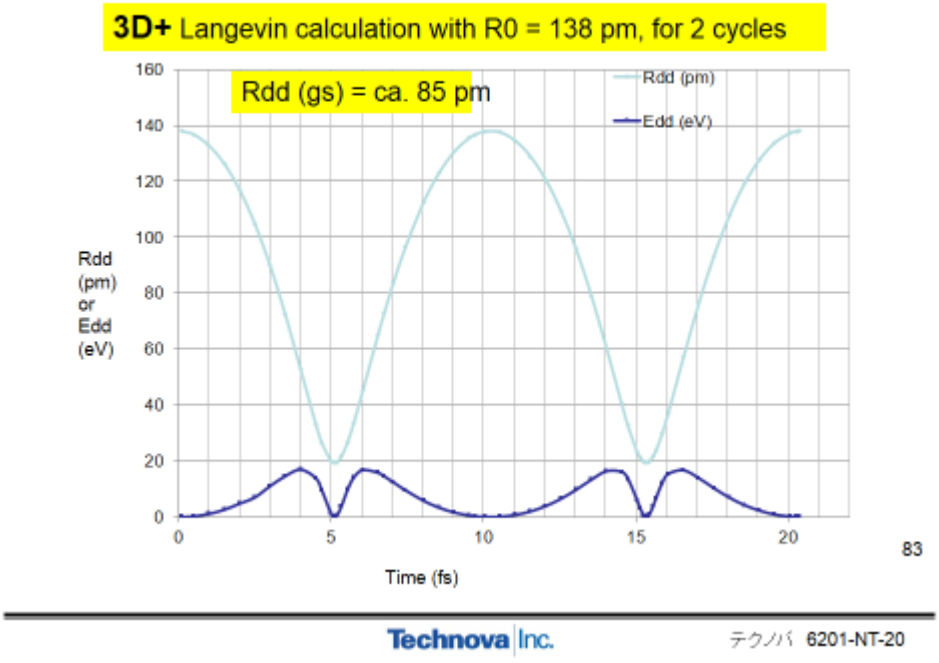

Fig.9: Initial two cycles of oscillation for 3D+ ionic molecule

Initial two cycles of simulated oscillation for 3D+ cluster is shown in Fig.9. It has the ground state with Rdd(gs) = 85 pm which is in good agreement with the result of Schroedinger equation analysis [8]. When starting calculation with R0=138 pm, complete steady oscillation with same amplitude was attained after about 500 oscillations. Changing R0 value around 138 pm, we have found almost the same

converging oscillation mode that is regarded as ground state.

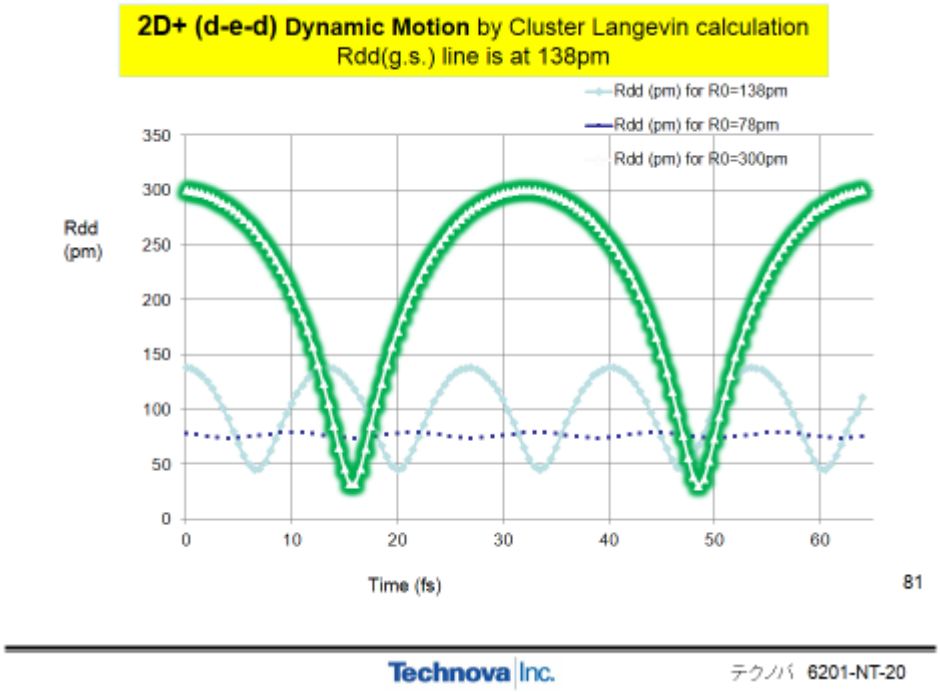

Fig.10: Initial two cycles of oscillation for 3D+ cluster started with R = 300 pm

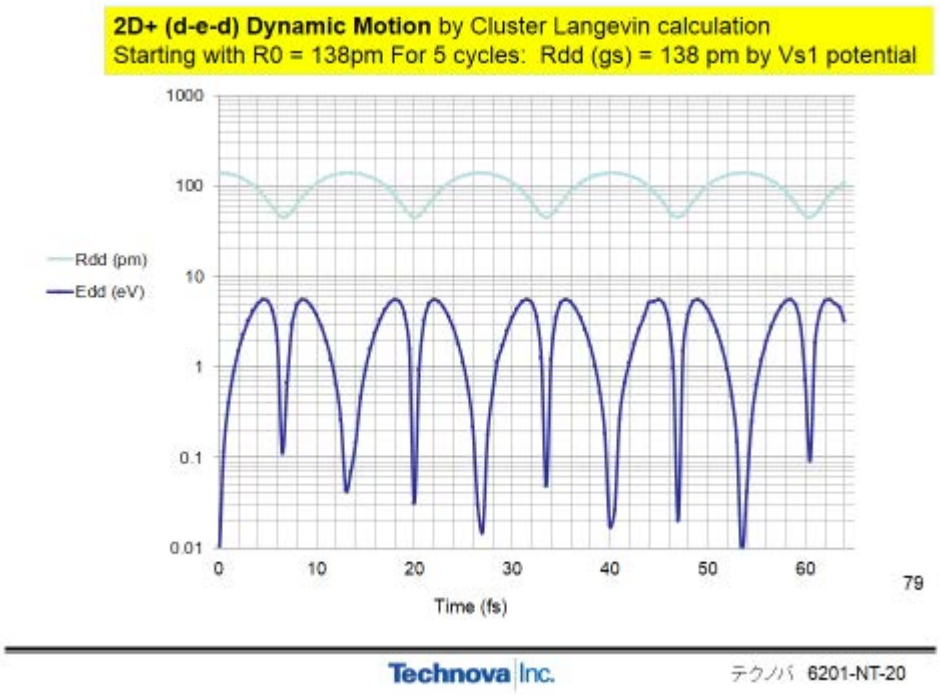

Fig.11: Initial 5 cycles of oscillation motion for 2D+(d-e-d) ionic molecule, started with R0 = 138 pm

The simplest cluster in the present paper is a d-e-d three body system. The first two cycles by starting with R0 = 300 pm is shown in Fig.10. Comparison is made with starting conditions of R0 = 138 pm and 78 pm. By random sampling of starting conditions we obtain corresponding oscillation curves. The ensemble average of curves will give the ground state solution. We know the ground state Rdd(gs) = 138 pm, as already discussed in Fig.1. Initial 5 cycles of oscillating motion of 2D+ (d-e-d) are plotted in Fig.11 for variation of Rdd(t) and relative kinetic energy of d-d pair.

The next interesting three body system is a muonic d-d molecule. When a muon sticks to a D_2 molecule, how does the time-dependent motion of dμd system look like? We used trapping potential of Vs1(50,2) that is known to be almost equivalent to Vs1(207,1) [3]. Using the starting value R0 = 74pm, simulation by the present code has given an interesting first oscillation cycle curves as shown in Fig.12. After about 2.7 fs, there happens very sharp valley of Rdd(t) curve and local maximum of relative d-d kinetic energy curve, the extended figure of which is drawn in Fig.13. The local minimum d-d distance there is Rdd = 0.2 pm and the local maximum relative d-d kinetic energy is ca. 3.0 keV. Next local maximum d-d distance after the first oscillation cycle is Rdd = ca. 52 pm which is smaller than the starting value of 74 pm; namely the system is condensing.

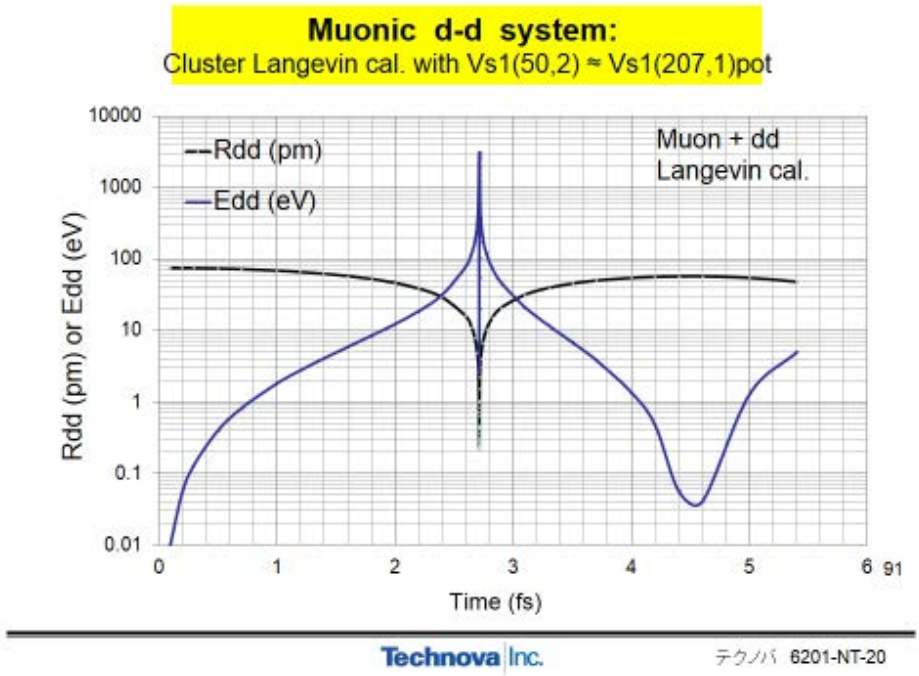

Fig.12: The initial one cycle of oscillation motion of muonic d-d molecule after sticking of muon onto a D_2 molecule.

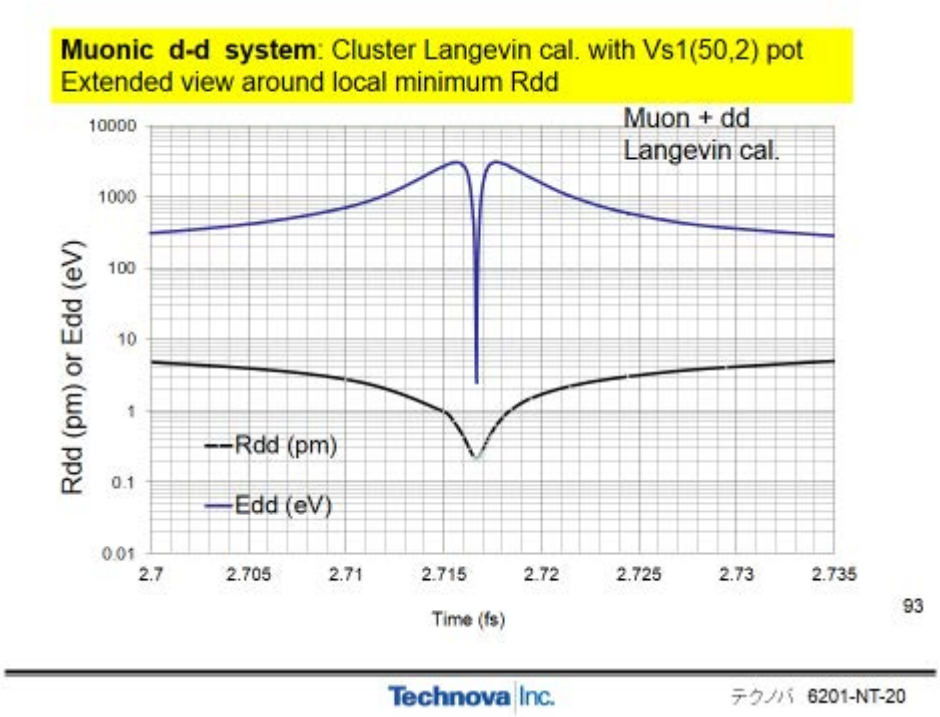

Fig. 13: Extended graph of Fig.12, for time interval around 2.7 fs

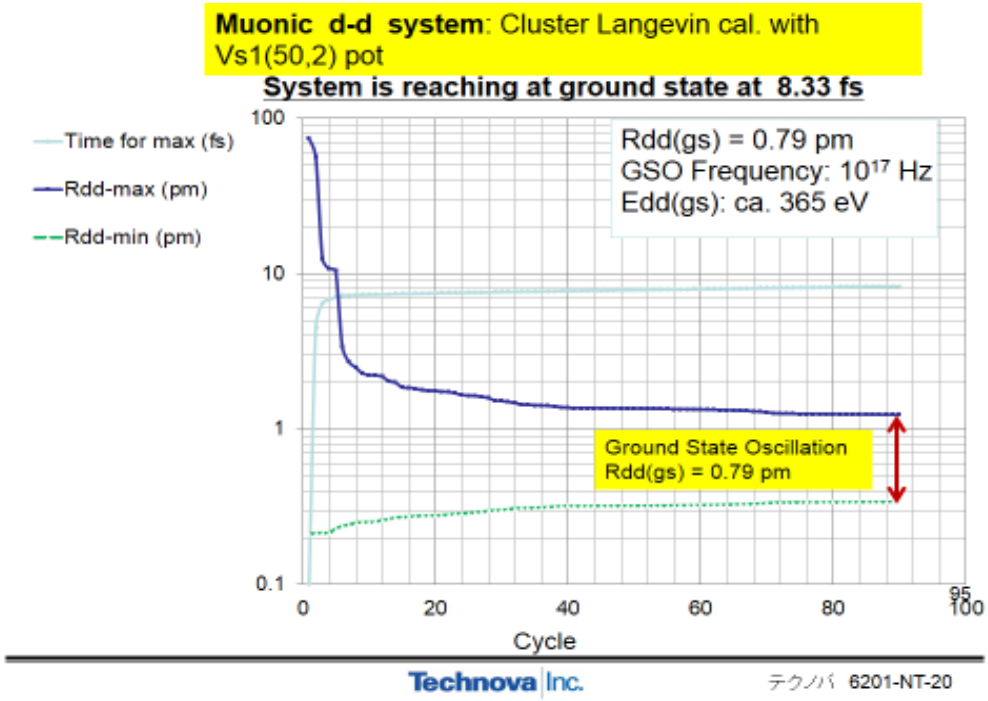

Fig.14: Condensing behavior of muonic d-d molecule after sticking of muon onto D_2 molecule. Changing starting R0 values around 100-50 pm does not effect on the converging 'ground' state.

For succeeding cycles of simulation, local maximum values of Rdd(t) decrease and local minimum values of Rdd(t) slowly increases as shown in Fig.14. After about 80 cycles of oscillation, it looks converging to an asymptotic oscillation that is regarded as the ground state of muonic d-d molecule with Rdd(gs) = 0.79pm. The ground state oscillation frequency is ca. 1.0E+17 Hz and the ground state relative d-d kinetic energy is estimated as ca. 365 eV which is a double score of the previously estimated value 180 eV by the QM variational calculation with Gaussian wave function (Rdd(gs) was 0.805 pm in that case) [9]. In the QM variational calculation [3, 9], we used a reduced mass for a d-d pair to be 1.0, while the mass of d in the present QM Langevin code is 2.0. Therefore the double score is understandable as the difference in conversion from the center-of-mass system to the laboratory system.

Now we come back to a known standard case of D_2 molecule. We know the mathematical functions [4, 5] in Vs2(1,1) potential for trapping D_2 molecule have difficulty in numerical calculation of its derivative (field-force form) to apply to QM Langevin calculation. However, we find that Vs1(1,1.41) potential has very close curve to that of Vs2(1,1) as compared in Fig.15. Therefore, we can simulate an approximate dynamic motion of D_2 molecule by the present code with use of Vs1(1, 1.41) potential. The initial two cycles of oscillation motion are drawn in Fig.16.

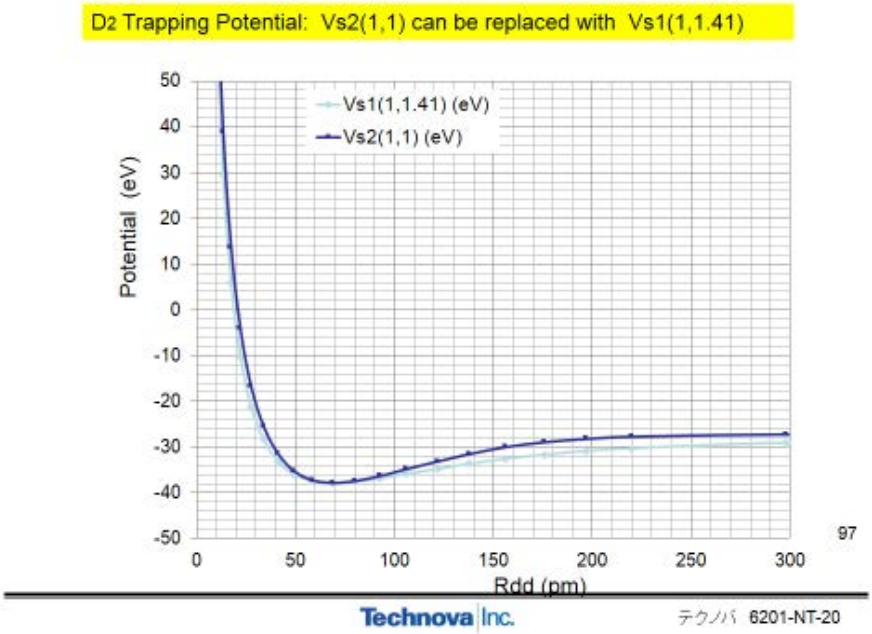

Fig.15: Vs1(1, 1.41) potential behaves closely to that of Vs2(1,1) potential of D_2 molecule

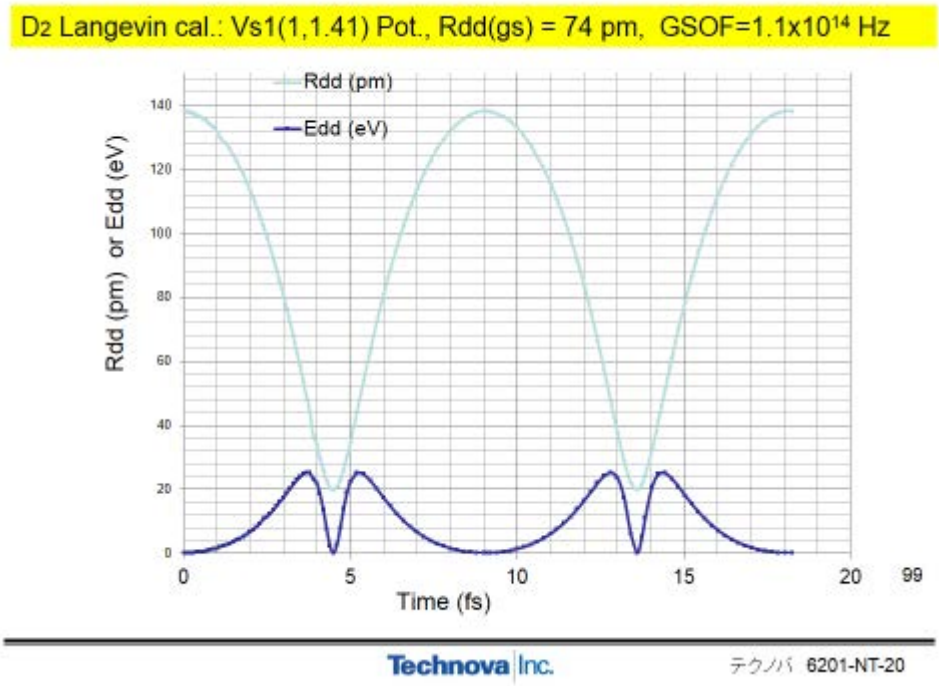

Fig.16: Initial two cycles of oscillation motion for D_2 molecule

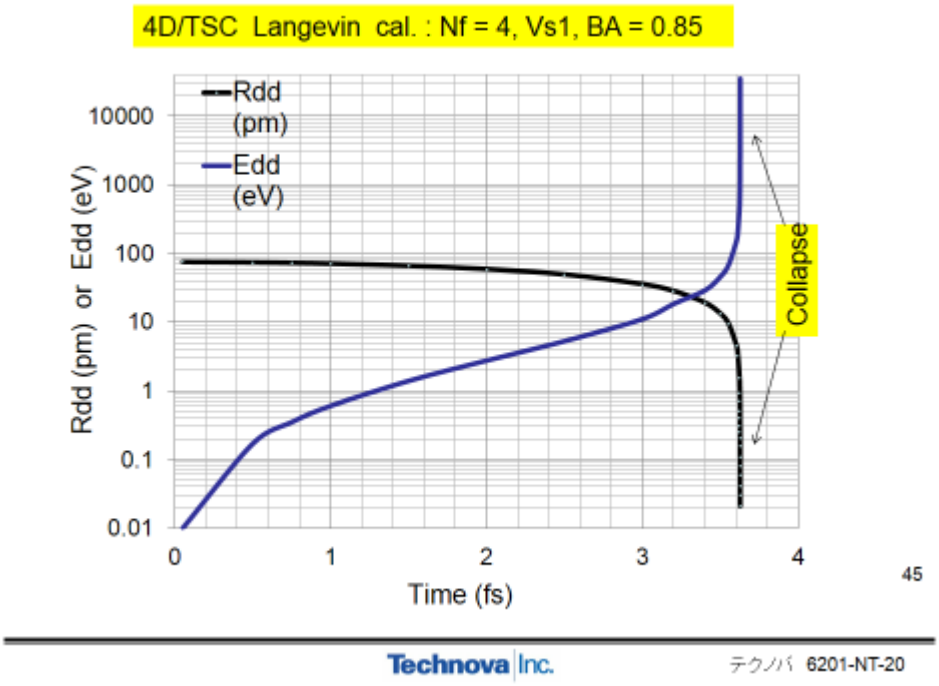

Fig.17: Condensation and collapse of 4D/TSC as simulated by the present code with the new rule for face trapping potential component

3.2 **Condensation Collapse of D(H)-Cluster Polyhedron**

Now we argue on the results for larger D(H)-clusters than 3D under 3 dimensional symmetry (Platonic symmetry). We have already given three key parameters for various D(H)-clusters in Table-1. The result for 4D/TSC by the new rule of usage of Vs1(1,1) potential for its unit face of triangle d-d-d is shown in Fig. 17. The 4D-cluster collapses at around 3.6 fs after the TS formation, while it was after 1.4 fs by using the old rule in References [2, 3] which used Vs1(2,2) potential of 'bosonized electron pair' on d-e-e-d surface of cubic TSC configuration.

Fig.18 illustrates the feature of 6D(2-) Rhombic dodecahedron. It has 12 d-d edges (Ne = 12) and 8 triangle d-d-d faces (Nf = 8). The value of k is estimated by D. Rocha to be 18.45 keVpm. The results of simulation by the present code are shown in Figs. 19 and 20. It has given collapse after ca. 4.1 fs. Near collapsing time-interval, we had to use very fine time meshes as 0.000001 fs (1.0E-21 s) as shown in Fig.20. Such very small time meshes would have not been tried in the past molecular dynamics codes conventionally available: usually as (1.0E-18 s) would have been the smallest time mesh as far as tried. Therefore, usual molecular dynamics codes (or static Schroedinger equation analyses) should have missed the collapsing states of D(H)-clusters which have no static ground state eigen-values but transient condensing and collapse evolution.

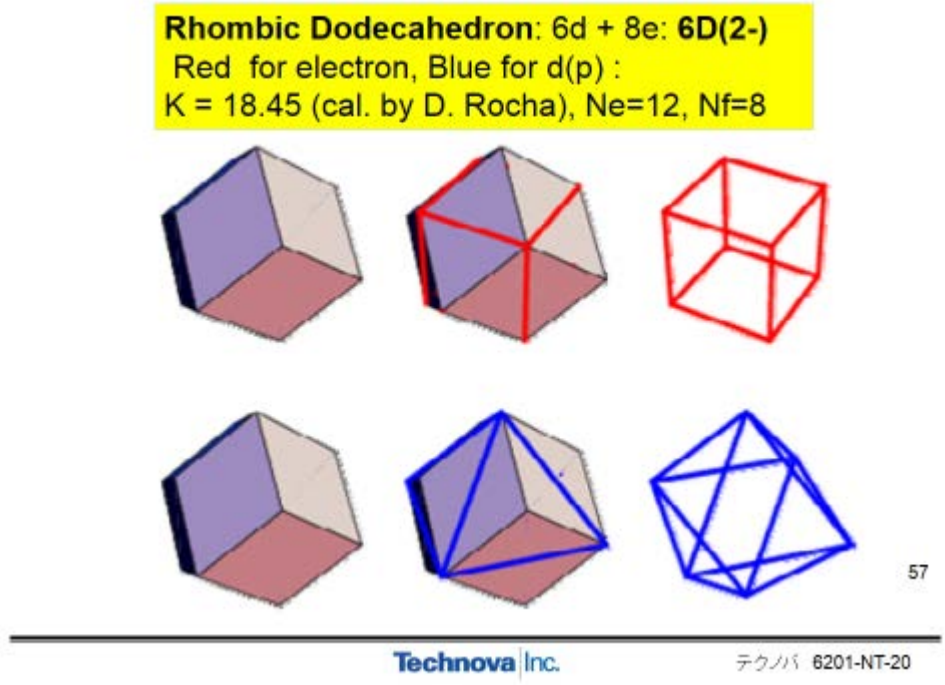

Fig.18: Rhombic dodecahedron is the polyhedron of 6D(2-)-cluster

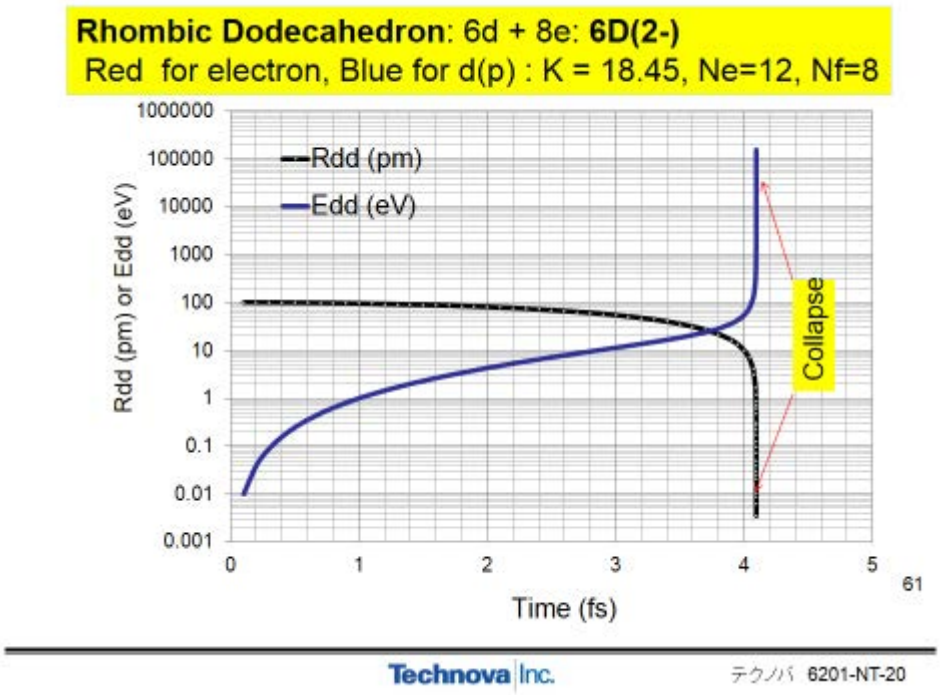

Fig.19: Simulated results of condensation motion of 6D(2-) Rhombic dodecahedron, getting to collapse after ca. 4.1 fs and maybe inducing 6D multi-body fusion

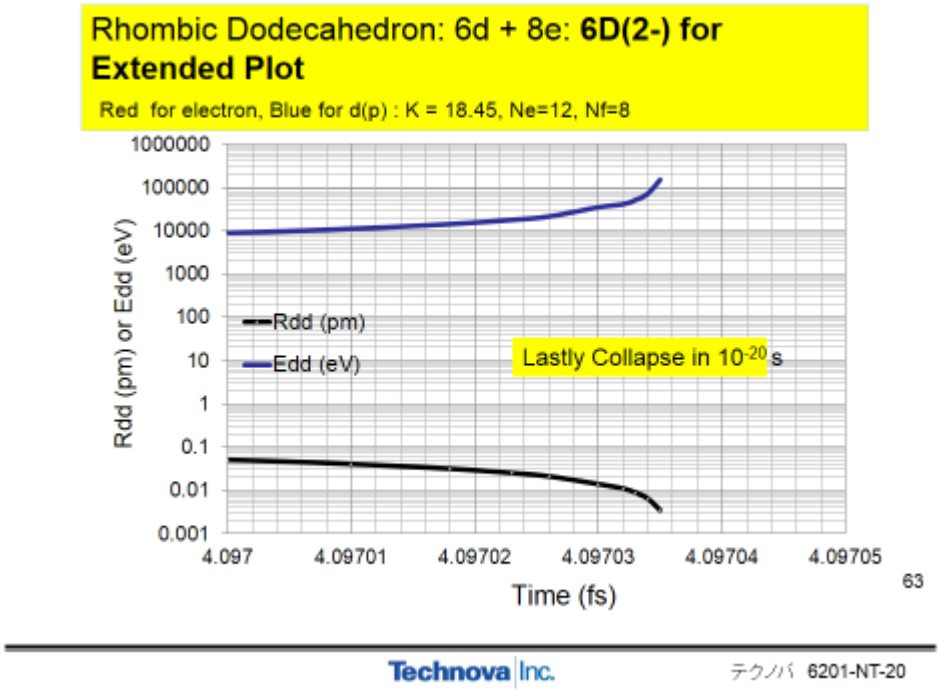

Fig.20: Extended graph of condensing evolution before collapse at around 4.097035 fs

When we exchange QM centers between electrons (red) and deuterons (blue) in Fig.18, we get 8D(2+) cluster of Rhombic dodecahedron. The result of simulation by the present code is shown in Fig.21. This 8D(2+) cluster may also collapse at ca. 3 fs after the cluster polyhedron formation.

Example for more larger D(H)-cluster is for the case of 20D(8+) cluster of Rhombic triacontahedron as its geometrical feature is illustrated in Fig.22. This 20D(8+) cluster may also collapse at around 6.5 fs after the cluster formation. What kind of strong interactions (so many body fusion?) will happen is the remained problem of nuclear physics consideration.

When we exchange QM centers between electrons (red) and deuterons (blue) of Fig.22, we get 12D(8-) cluster of Rhombic triaconrahedron. The simulation calculation for the system, as shown in Fig.24, does not make collapse but converges to steady oscillation of ground state, interestingly. We tried to find that some other polyhedral cluster as 6D(2-)/OSC does not collapse either.

To summarize the results of simulation for various clusters, in the view of collapse and possible multi-body nuclear interactions, Table-2 is conclusively obtained.

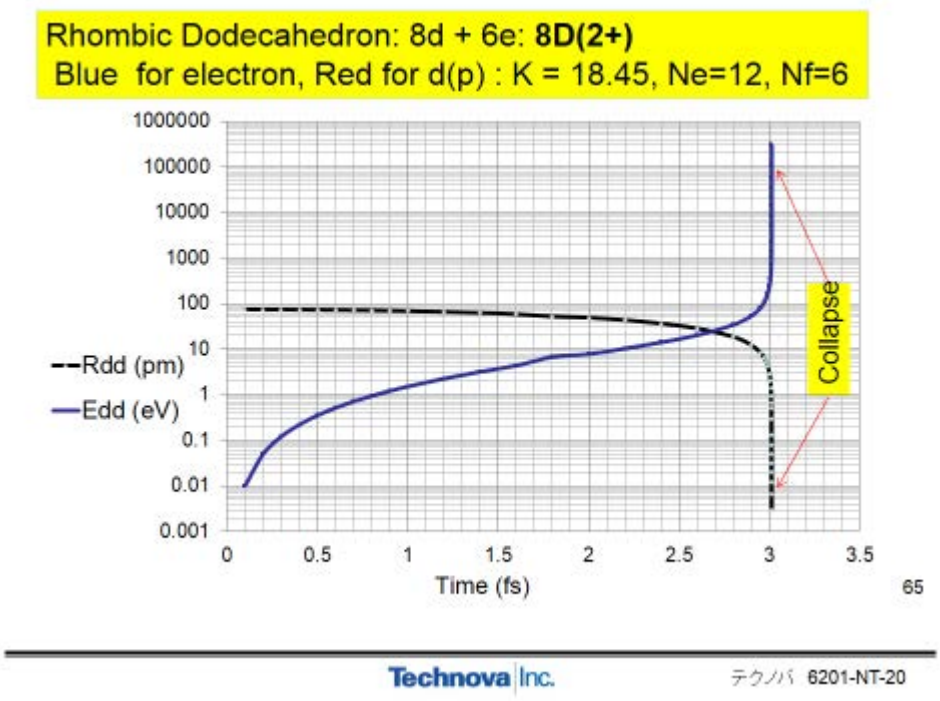

Fig.21: Results of simulation for condensation motion of 8D(2+) cluster

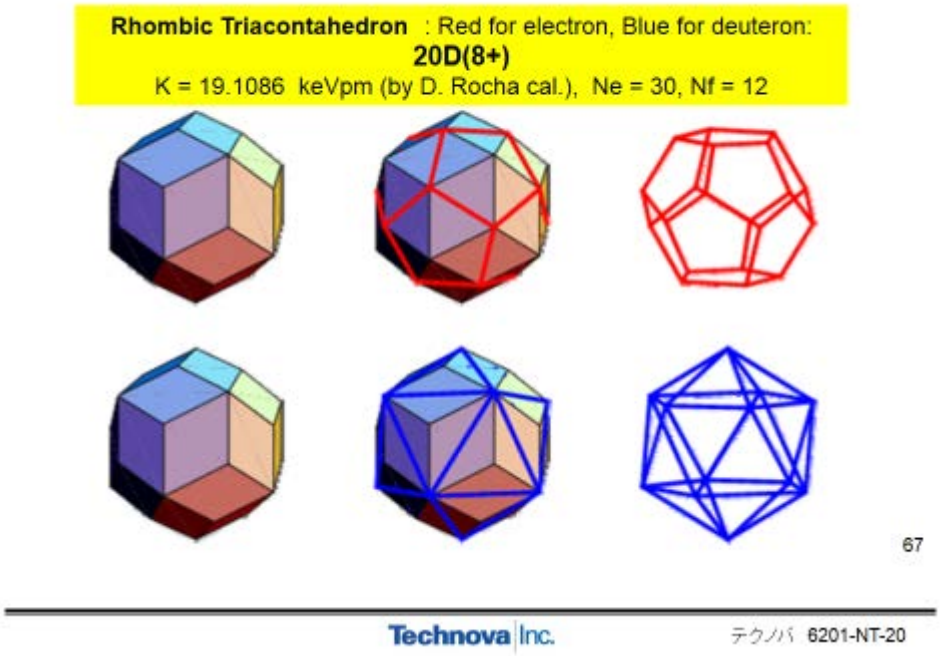

Fig.22: Geometrical feature of 20D(8+) cluster of Rhombic triacontahedron

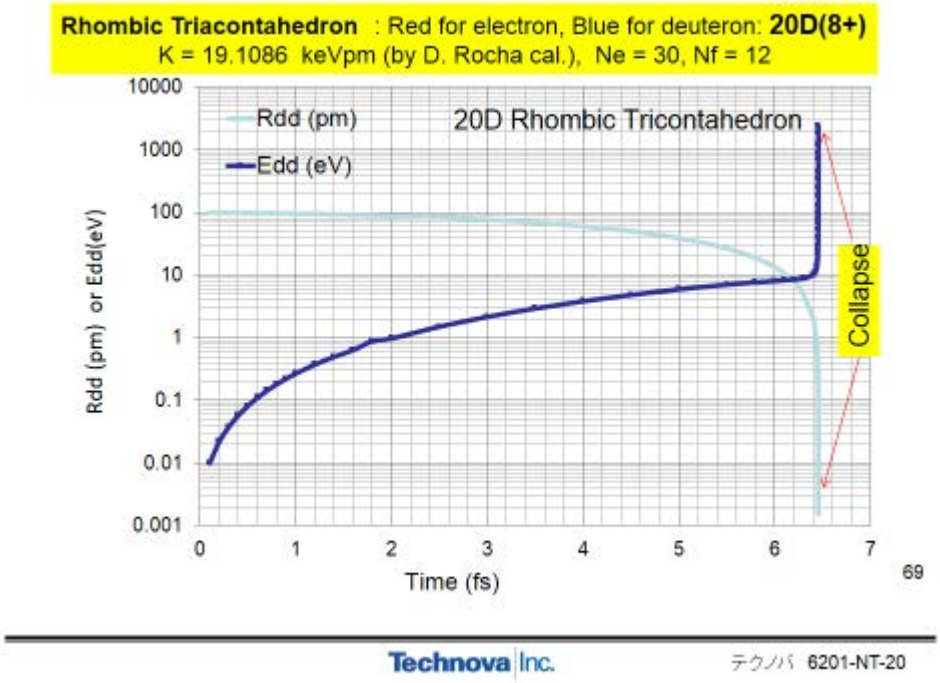

Fig.23: Results of simulation for 20D(8+) cluster of Rhombic triacontahedron

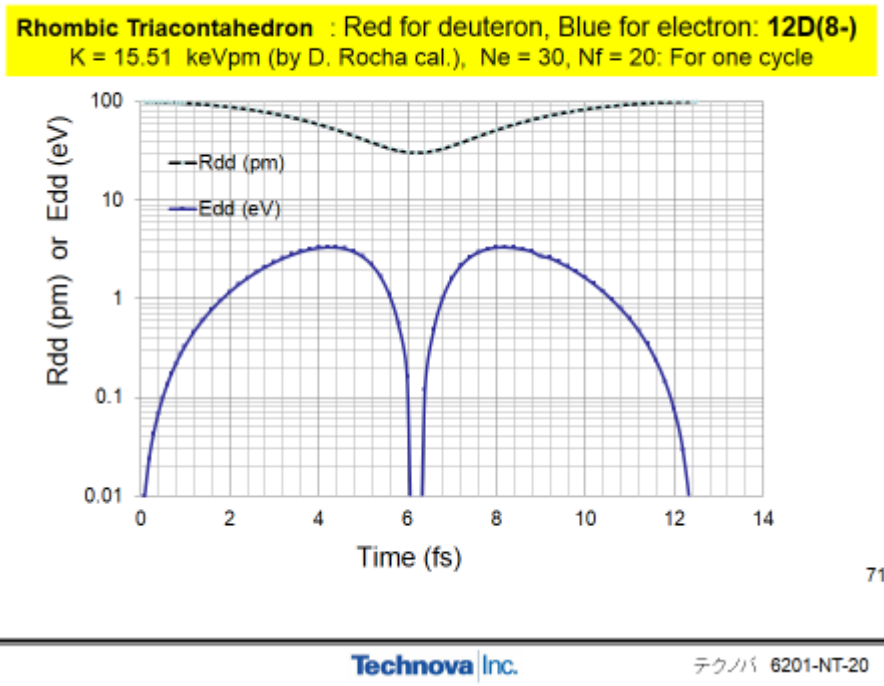

Fig.24: Results of simulation for 12D(8-) cluster of Rhombic triacontahedron

Table-2: Summary of condensation and collapse states for D-clusters;
Here RD denotes Rhombic dodecahedron and RT does Rhombic triacontahedron.

Summary of Results

Cluster Type	Collapse? (Rdd-min ≦10 fm)	Rdd (gs)	Remarks
d-e-d (2D+)	N	138 pm	
d-μ-d	N	0.79 pm	DD fusion in 0.1ns
3D+	N	85 pm	
4D/TS	Y		100% 4D fusion
6D/RD	Y		100% 6D fusion
8D/RD	Y		100% 8D fusion or 4D fusion?
12D/RT	N	ca. 80 pm	
20D/RT	Y		What kind of fusion?

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3.3 **Simulation of EQPET D(H)-Clusters**

Because of the spin arrangement of electrons in D(H)-clusters of polyhedra, condensation motion may be somewhat different from above results for which the spin effect was not treated.

The anti-parallel arrangement of spins for counter-part electrons in polyhedron of D(H)-cluster, bosonized pseudo-particle state of coupled electrons were assumed in our previous study on D(H)-cluster condensation [5]. The typical bosonized pseudo-particle states of oriented electrons as assumed in reference [5] are illustrated in Fig.25.

Results of simulation calculations for EQPET clusters by the present code are shown in Figs. 26 through 29. In many cases, EQPET clusters have very diminished size ground states as summarized in Table-3. Since these diminished size states as ground states have infinite life time and very close d-d (or p-p) inter-nuclear distances, reaction rates by strong (even weak) interactions may become significantly large to be able to argue on the possibility of condensed matter nuclear reactions aka cold fusion.

In this paper, example figures for H-systems are not specifically shown. However condensation speed is inversely proportional to mass and all figures may be rescaled for the case of H-clusters.

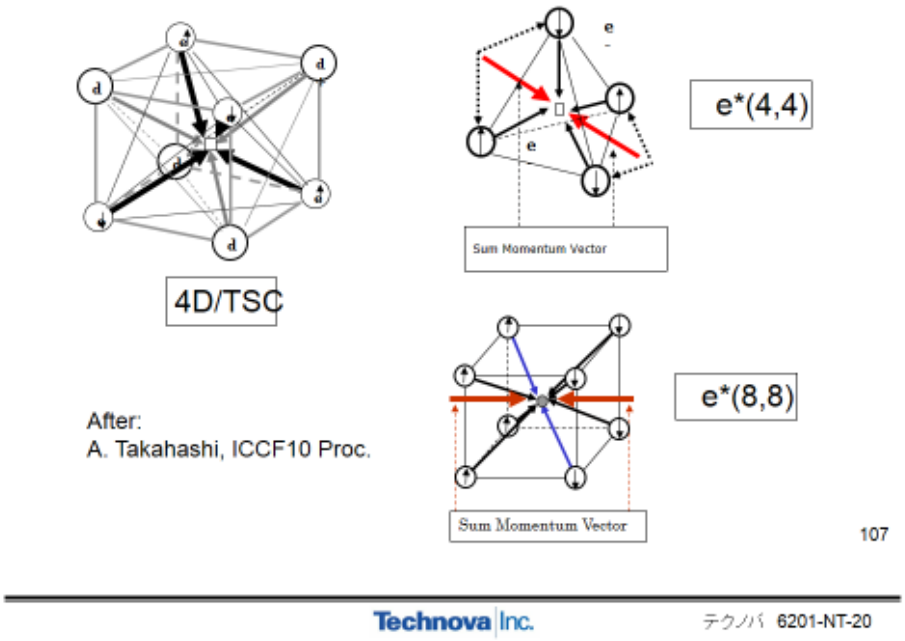

Fig.25: Assumed bosonized quasi-particles of oriented electrons

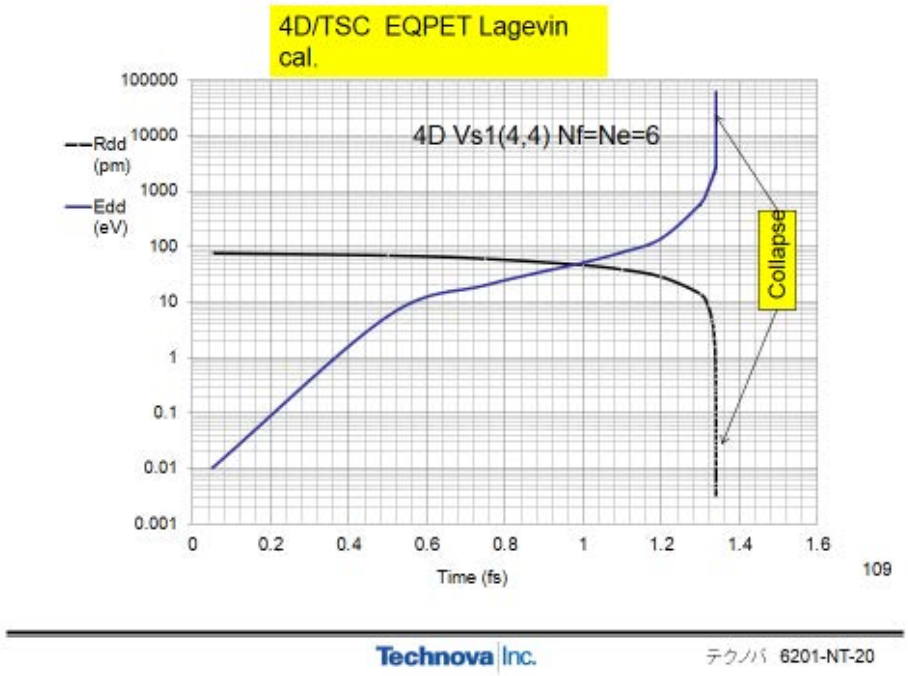

Fig.26: Results of simulation for 4D/TSC cluster with Vs1(4,4) EQPET potential

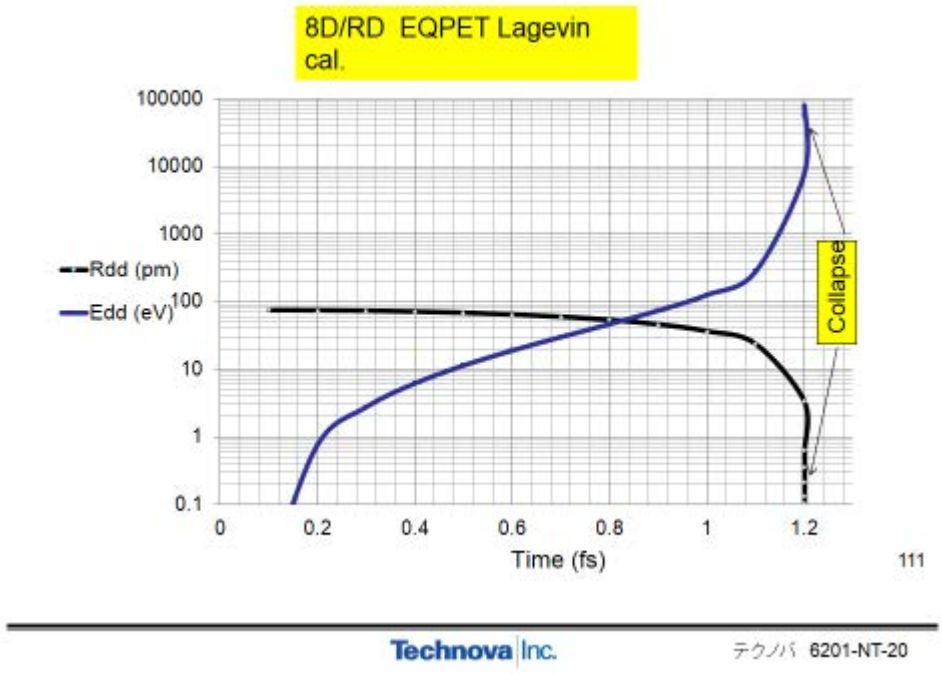

Fig.27: Results of simulation for EQPET 8D/RD cluster

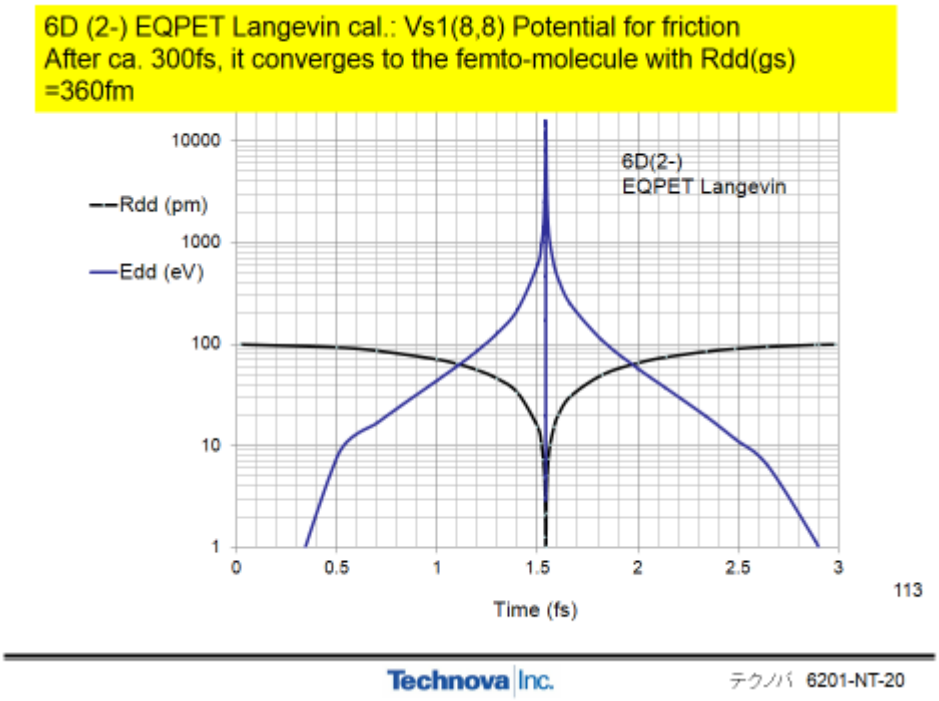

Fig.28: Results of simulation for EQPET 6D(2-) cluster with Vs1(8,8) potential, having no collapse but converged ground state of diminished size cluster (Rdd(gs) = 125 fm)

Table-3: Summary of converged ‘ground’ sates for EQPET clusters

Calculated convergence-to-Femto-Molecule by EQPET Langevin mode (Use dim 200000): by D.R.

Cluster Type	e* (m, Z)	Rdd (gs) (fm)
4D/TSC	(4,4)	None (collapse)
6D(2-)/OSC	(8,8)	360
6D(2-)/RD	(8,8)	125
6D(n)/RD	(6,6)	300 (Nf=12)
12D(8-)/RT	(20,20)	42
20D(8+)/RT	(12,12)	150

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A typical example of simulation for such EQPET clusters is the cases of 4D/TSC with Vs1(4,4) trapping potential and 8D/RD neutral-cluster with Vs1(8,8) trapping potential. Results of simulation on condensation/collapse motion by the present code are shown in Figs. 26 and 27.

4. Concluding Remarks

A generalized PC computer code written by Basic language has been developed for making simulation calculations on very time-sensitive dynamics behavior of polyhedral D(H) clusters which transient behavior is recognized very important according to the physical mechanisms of condensed matter nuclear reactions aka cold fusion.

For realizing the frictional/constraint force components caused by the quantum mechanical motion of electrons in D(H)-cluster, the well-studied Coulombic trapping potential Vs1(1,1) of three body system (d-e-d or p-e-p) was used as a unit of particle trapping force per a regular triangle d-d-d (or p-p-p) surface of D(H)-cluster polyhedron assuming the 3 dimensional symmetry (Platonic symmetry). Evaluating three key parameters as k-value of centripetal Coulombic force of cluster, number of d-d (or p-p) edges Ne and number of regular triangle surfaces for individual D(H)-cluster, the programmed D(H)-cluster Langevin code can be run for simulation of very precise time-dependent behavior of condensation and sometimes collapsing states.

Time steps of numerical Verlet run must be very fine as 1.0E-21 s to find very rapidly collapsing states. Such extremely small time mesh dynamics may be new in molecular/cluster-forming dynamics codes as given conventionally. Usual time mesh calculations with a few fs or even few as time mesh should miss easily the collapse states due to the time-averaging or error accumulation in time-step sequences of numerical calculation. Of course, the eigenvalue approach by the static Schroedinger equations cannot resolve such very fast transient behavior. The developed QM-Langevin method is a unique tool that should be very usable in studying underlying dynamic mechanisms of condensed matter nuclear reactions aka cold fusion.

Summary of most important consequences in this respect of cold fusion is given in Table-2. We may conclude the polyhedral D(H) cluster such as 4D(H)/TS, 6D/RD, 8D/RD, 20D/RT have something to do with inducing dreamy cold fusion events.

Acknowledgment: Kind support to this work by Technova colleagues (A. Kitamura, R.

Seto and Y. Fujita) is appreciated.

References:

[1] Akito Takahashi: The basics of deuteron cluster dynamics as shown by Langevin equation, American Chemical Society *LENRSB (Low Energy Nuclear Reaction Source Book)* 2 (2009) 193-217

[2] Akito Takahashi and Norio Yabuuchi: Study on 4D/TSC condensation motion by non-linear Langevin equation, American Chemical Society *LENRSB* 1 (2008) 57-83

[3] Akito Takahashi: Physics of Cold Fusion by TSC Theory, *J. Physical Science and Application*, 3(3) (2013) 191-198

[4] L. C. Pauling, A. Wilson: Introduction to Quantum Mechanics with Applications to Chemistry, McGraw-Hill, New York, 1935

[5] Akito Takahashi: JCMNS, Vol.1, 62-85 (2007)

[6] A. Takahashi, D. Rocha: Proc. JCF-13, pp.10-31 (2013), http://jcfrs.org/file/jcf13-proceedings.pdf

[7] Akito Takahashi: Nuclear Products of Cold Fusion by TSC Theory, Proc. ICCF18, to be published in JCMNS (see http://vixra.org/abs/1309.0072 also)

[8] I. D. Petsarakis, et al.: J. Chem. Phys., 87 (1983) 3806

[9] Akito Takahashi: Kinetic Reaction Energy of Cold Fusion, JCF-12-7, Proc. JCF-12, pp. 67-76 (2013), http://jcfrs.org/file/jcf13-proceedings.pdf

Appendix: D(H)-Cluster Langevin Program

1 ! Cluster Langevin Code (written by Akito Takahashi, revised on April 11 2013)

2 ! Instruction: Time-dependent motion of d-d (or p-p) distance for a polyhedral deuteron(d) or proton(p) cluster is calculated.

3 ! Source Literature: Akito Takahashi: The Basics of Deuteron-Cluster Dynamics as Shown by a Langevin Equation, ACSLENRSB Vol.2, Chapter 11, pp.193-217, 2009

4 ! the second literature: A. Takahashi, N. Yabuuchi, Study on 4D/TSC Condensation Motion by Non-Linear Langevin Equation, ACSLENRSB Vol.1, pp.57-83, 2008

5 ! Correction in the second literature: In Appendix, (A-4) minus is missing for K, (A-9) minus should be removed for K'

```
11 ! ms: mass number (cf. electron) of electronic quasi-particle, Z: relative charge (cf. electron) of EQ
12 ! BA: bias factor by <f(t)> for the main centripetal Coulombic force: BA=0.91 is recommended for most cases.
16 input BA
17 print using "BA=%.####" :BA
20 input ms
30 print using "ms=%.####" :ms
40 input Z
50 print using "Z=%.####" :Z
55 ! EK is k-value (keVpm) for centripetal force, EK=3.65 for 3D+, EK=11.85 for 4D/TSC, EK=10.97 for 6D(2-)
56 ! FNf is the number of effective faces of d(or p)-polyhedron: FNf=4 for 3D+, FNf=4(for Vs1(1,1)) or 6(for Vs1(2,2) or Vs1(4,4)) for 4D, Nf=8 (for Vs1(1,1)) for 6D
57 ! FNe is the number of nearest d-d edges: FNe=3 for 3D+, FNe=6 for 4D, FNe=12 for 6D
58 ! fmrev is the inverse of d (or p)-mass: 4.77E4 for deuteron, 2*4.77E4 for proton (See the second literature).
59 ! R0 is the starting d-d distance in pm unit.
60 ! Please write-in the following parameters in line 62-66
62 LET    EK=11.85
63 LET    FNf=6
64 LET    FNe=6
65 LET    fmrev = 4.77E4
66 LET R0=74.0
69 input TDT
70 print using "DT=%.#####" :TDT
100 DIM RDD(2000), R(2000), T(2000), V(2000), VS1(2000), FCOND(2000), BALANCE(2000), G(2000), ED(2000), DT(2000)
110 ! T is in (fs), R and RDD are in (pm), V is in (pm/fs), VS1 and ED are in (keV), FCOND and BALANCE are in (pm/fs/fs)
210 LET V(1)=1.0
215 LET T(1)=0.0
218 LET R(1)=V(1)*TDT
220 LET IMAX=2000
230 LET I=1
300 do while I<IMAX
```

```
305     LET DT(I)=TDT
320     LET RDD(I)=R0-R(I)
321     if RDD(I)<=20 then LET DT(I)=0.1*TDT
322     if RDD(I)<=5 then LET DT(I)=0.01*TDT
323     if RDD(I)<=1 then LET DT(I)=0.001*TDT
324     if RDD(I)<=0.5 then LET DT(I)=0.0001*TDT
325     if RDD(I)<=0.05 then LET DT(I)=0.00001*TDT
315     if RDD(I)<=0.001 then LET RDD(I)=0.001
330     LET y=ms*Z*RDD(I)/52.9
340     LET FJ=0.0272*Z^2*ms*(-1/y+(1+1/y)*exp(-2*y))
350     LET FK=-0.0272*Z^2*ms*(1+y)*exp(-y)
360     LET FD=(1+y+y^2/3)*exp(-y)
365     LET VS1(I)=-0.0136*Z^2*ms+1.44/RDD(I)+(FJ+FK)/(1+FD)
370     LET FJD=(5.14E-4)*Z^3*ms^2*((1.0-exp(-2*y))/y^2-2*(1.0+1/y)*exp(-2*y))
380     LET FKD=(5.14E-4)*Z^3*ms^2*y*exp(-y)
390     LET FDD=-(6.3E-3)*(y+y^3)*exp(-y)
400     LET DVS=-1.44/RDD(I)^2+((FJD+FKD)*(1+FD)+(FJ+FK)*FDD)/(1+FD)^2
410     LET BALANCE(I)=(FNf*fmrev/FNe)*DVS
420     LET FCOND(I)=(EK*fmrev/FNe)/RDD(I)^2
430     LET G(I)=BA*FCOND(I)+BALANCE(I)
500     ! Verlet Solution
510     LET R(I+1)=R(I)+V(I)*DT(I)+0.5*G(I)*DT(I)^2
512     LET RDD(I+1)=R0-R(I+1)
513     if RDD(I+1)<=0.001 then LET RDD(I+1)=0.001
515     LET y=ms*Z*RDD(I+1)/52.9
516     LET FJ=0.0272*Z^2*ms*(-1/y+(1+1/y)*exp(-2*y))
517     LET FK=-0.0272*Z^2*ms*(1+y)*exp(-y)
518     LET FD=(1+y+y^2/3)*exp(-y)
519     LET FJD=(5.14E-4)*Z^3*ms^2*((1.0-exp(-2*y))/y^2-2*(1.0+1/y)*exp(-2*y))
520     LET FKD=(5.14E-4)*Z^3*ms^2*y*exp(-y)
521     LET FDD=-(6.3E-3)*(y+y^3)*exp(-y)
522     LET DVS=-1.44/RDD(I+1)^2+((FJD+FKD)*(1+FD)+(FJ+FK)*FDD)/(1+FD)^2
523     LET G(I+1)=BA*(fmrev*EK/FNe)/RDD(I+1)^2+(fmrev*FNf/FNe)*DVS
530     LET V(I+1)=V(I)+(DT(I)/2)*(G(I+1)+G(I))
540     LET ED(I)=(0.5/fmrev)*V(I)^2
590     if RDD(I)<=0.001 then LET IMAX=I
```

```
595       if RDD(I)<=0.001 then LET RDD(I)=0.001
600       if RDD(I)<=0.001 then exit DO
650       LET I=I+1
700 loop
800 ! Print Outputs
810 LET AA$="T(fs) "
820 LET AB$="RDD(pm) "
830 LET AC$="v(pm/fs) "
840 LET AD$="ED(keV) "
850 LET AE$="Vs(keV) "
860 LET AF$="Fcond(pm/fs/fs) "
870 LET AG$="Balance(pm/fs/fs) "
880 LET AH$="G(pm/fs/fs)"
890 print AA$&AB$&AC$&AD$&AE$&AF$&AG$&AH$
910 LET I=1
920 LET T(1)=TDT
950 do while I<=IMAX-1
955       LET T(I+1)=T(I)+DT(I)
960         print using "-%.#######^^^^ -%.###^^^^ -%.###^^^^ -%.###^^^^ -%.###^^^^
-%.###^^^^ -%.###^^^^ -%.###^^^^" : T(I), RDD(I), V(I), ED(I), VS1(I), FCOND(I),
BALANCE(I), G(I)
970       LET I=I+1
1000 loop
1100 stop
       END
```

Note: Basic software is available at:

- The source of BASIC EXE under use in our PCs is downloadable from here:
- http://hp.vector.co.jp/authors/VA008683/basicw32.htm
- The instruction is in Japanese.
- **BASIC761** : you may right-click it and download.