

# Basics of Deuteron-Cluster Dynamics by Langevin Equation

Akito Takahashi (Prof. Emeritus, Osaka University) Technova Inc. To be presented at ACS2009 NET Symposium, Salt Lake City March 2009

## 1. Outline

- Generation and condensation of 4D/TSC as seed of clean fusion in condensed matter was previously studied by Langevin equation
- Basics of Langevin Equation for D-cluster is treated in this study
- Known D-systems: D, D2, D2<sup>+</sup>, D3<sup>+</sup>
- 4D/TSC and 6D/OSC

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Barrier factors and fusion rates

#### Result of Dynamic Condensation of 4D/TSC by Langevin Equation



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#### Case-1

Model for generating 4D/TSC (t=0) cluster in excited state dynamics of O-site Deuterons in PdD lattice, where D behaves as a harmonic oscillator



Figure 8. Image of lattice potential change by D-phonon excitation.

Under the stimulation of D-phonon excitation in PdDx (suppose locally x=1) lattice, transient 4D-cluster will be formed with certain probability [28]. We know the trapping periodical potential height for D in PdDx lattice is about 0.22 eV, and we use kinetic energy of deuteron  $E_d = 0.22 \text{eV}$  for numerical estimation in the following. To keep charge neutral sate in average, orthogonal combination of two transient D<sub>2</sub> molecules will be formed when 4 deuterons are squeezing from O-sites to central T-sites taking (conveying) 4 electrons from Pd 4d-shell (conduction band), as shown in Fig.1, under the TSC condition and the cluster of 4D<sup>+</sup>s and 4e<sup>-</sup>s makes a regular cube as shown in Fig.2.



Figure 1. Tetrahedral condensation of deuterons in PdD lattice

#### **Tetrahedral Condensation of Deuterons in PdDx**



A. Takahashi: Proc. ICCF10, pp.809-818, World Scientific PC, 2006

#### Feature of QM Electron Cloud



b) D<sub>2</sub> molecule (stable):  $\Psi_{2D} = (2+2\Delta)^{-1/2} [\Psi_{100}(r_{A1}) \Psi_{100}(r_{B2}) + \Psi_{100}(r_{A2}) \Psi_{100}(r_{B1})] X_{s}(S1,S2)$ 

## Elaboration of 4D/TSC Models

- A. Takahashi: Deuteron cluster fusion and related nuclear reactions in metal-deuterium/hydrogen systems, *Recent. Res. Dev. Physics*, 6(2005)pp.1-28
- A. Takahashi: A theoretical summary of condensed matter nuclear effects, Proc. Siena05 Workshop, to be published in *JCMNS (2007)*
- A. Takahashi, N. Yabuuchi: Condensed matter nuclear effects under Platonic symmetry, Proc. ICCF13
- A. Takahshi, N. Yabuuchi: Study on 4D/TSC condensation motion by non-linear Langevin equation, Proc. New Energy Technologies, ACS, 2007 (published from Oxford U. Press, August 2008)
- And others in Proceedings of ICCF11-14.



This work: Milestones for solving the problem

- So many body problem: 4d +4x(D1selectron)+ 4x10x(Pd 4d-shell electron)+4Pd + surrounding lattice atoms
- Platonic Symmetry helps the problem make simpler
- Formulate one-dimensional Langevin equation for D-cluster dynamics

One-Dimensional Langevin Equation for Molecule with Platonic Symmetry

- Formulate Langevin Equation with onedimensional Rdd (d-d distance).
- Treat electron wave by combination of "dede" or "dde" type potentials.
- Solve Langevin Equation for D-clusters with Platonic symmetry for deuterons and electrons: D, D2, D2<sup>+</sup>, D3<sup>+</sup>, 4D/TSC, 6D<sup>--</sup> /OSC.

# 2: D(H)-atom

1S-wave function

$$\Psi_{100}(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

System Coulomb Energy

$$\langle \Psi_{100} | E_{C-D} | \Psi_{100} \rangle = \int_0^\infty (-e^2 / r) \Psi_{100}^2 4\pi r^2 dr = -1.44 / r$$

With r = Bohr radius (52.9 pm), we get

$$\langle E_{C-D} \rangle = -27.2 eV$$

# D(H)-atom-II

 Total system energy is given by Hamiltonian integral:

$$\langle H \rangle = \langle \Psi_{100} | H | \Psi_{100} \rangle = \langle \Psi_{100} | -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{r} | \Psi_{100} \rangle = E_0 = -136eV$$

$$\langle H \rangle = \langle E_k \rangle + \langle E_{C-D} \rangle$$
Kinetic energy Coulomb energy
$$\langle E_k \rangle = \frac{1}{2} m v^2 (r = a_B) = \frac{e^2}{2r} = 13.6eV$$

### **D-Atom: Point-Sphere Coupling**



# 2.2) D-atom Langevin Equation

Regarding QM average = Ensemble Av.

 $\langle G \rangle_{ensemble} = \langle \Psi | G | \Psi \rangle$ 

$$m_{e} \frac{d^{2} R_{de}}{dt^{2}} = -\frac{e^{2}}{\left[R_{de}\right]^{2}} + \frac{m_{e} v_{e}^{2}}{R_{de}} + f(t)$$

$$m_e \frac{d^2 \langle R_{de} \rangle}{dt^2} = -\left\langle \frac{e^2}{R_{de}^2} \right\rangle + \left\langle \frac{m_e v_e^2}{R_{de}} \right\rangle = 0$$

$$m_e \frac{d\langle R_{de} \rangle}{dt} = F(T) = \int_0^T f(t) dt = \langle f(t) \rangle = 0$$

Due to the ergodic process

$$\left\langle R_{de}\right\rangle(t) = R_0 = R_B = 52.9\,pm$$

$$\left\langle E_{KE} \right\rangle = \frac{1}{2} m_e \left\langle v_e^2 \right\rangle = \frac{e^2}{2R_B} = 13.6eV$$
$$\left\langle E_C \right\rangle = -\frac{e^2}{R_B} = -27.2eV$$

$$\langle H \rangle = \langle E_{\rm KE} \rangle + \langle E_{\rm C} \rangle = -13.6 eV$$

Balance of centripetal And centrifugal force

Mean Electron Kinetic Energy = 13.6 eV ; 332 pm Wave Length=  $2 \pi R_B$ 

## 3. D<sub>2</sub> molecule

• System wave function:

$$\Psi_{2D} = \frac{1}{\sqrt{(2+2\Delta)}} \Big[ \Psi_{100}(r_{A1}) \Psi_{100}(r_{B2}) + \Psi_{100}(r_{A2}) \Psi_{100}(r_{B1}) \Big] X_s(S1, S2)$$

System Energy at ground state

$$\left\langle \Psi_{2D} \middle| H \middle| \Psi_{2D} \right\rangle = -35.1 eV$$

System Coulomb Energy: Semi-Classical model

$$\left\langle E_{C-2D} \right\rangle = 4\left(-\frac{e^2}{a_B}\right) + 2\left(\frac{e^2}{\sqrt{2}a_B}\right) = -70.3eV$$

17.6 eV per e

**Electron Kinetic E** 

 $\langle E_{ke-2D} \rangle = \langle H_{2D} \rangle - \langle E_{C-2D} \rangle = 70.3eV - 35.1eV = 35.2eV$ 

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## **Quantum-Mechanical Ensemble-Averaging**

$$\langle G \rangle_{ensemble} = \langle \Psi | G | \Psi \rangle$$

Born-Oppenheimer Approximation; for D2 molecule:

$$\Psi(R_{dd}; r_{A1}, r_{A2}, r_{B1}, r_{B2}) = \Psi_{2D} \cdot X(R_{dd})$$

Electron Wave Function for D<sub>2</sub>:

$$\Psi_{2D} = \frac{1}{\sqrt{(2+2\Delta)}} \Big[ \Psi_{100}(r_{A1}) \Psi_{100}(r_{B2}) + \Psi_{100}(r_{A2}) \Psi_{100}(r_{B1}) \Big] X_s(S1, S2)$$

Deuteron Wave Function: Gaussian approximation:

$$X^{2}(R'_{dd}; R_{dd}(t)) = \frac{1}{\sqrt{2\pi\sigma^{2}}} \exp[-(R'_{dd} - R_{dd}(t))^{2}/(2\sigma^{2})]$$

#### D<sub>2</sub> Molecule Electron Localization; 1/2

$$\Psi_{2D} = \frac{1}{\sqrt{(2+2\Delta)}} \Big[ \Psi_{100}(r_{A1}) \Psi_{100}(r_{B2}) + \Psi_{100}(r_{A2}) \Psi_{100}(r_{B1}) \Big] X_s(S1, S2)$$

$$\left| (4\pi)^4 \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \Psi_{2D}^2(r_{A1}, r_{A2}, r_{B1}, r_{B2}) r_{A1}^2 r_{A2}^2 r_{B1}^2 r_{B2}^2 dr_{A1} dr_{A2} dr_{B1} dr_{B2} = 1 \right|$$

$$\int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \rho(r_{A1}, r_{A2}, r_{B1}, r_{B2}) dr_{A1} dr_{A2} dr_{B1} dr_{B2} = 1$$

$$\rho(r_{A1}, r_{A2}, r_{B1}, r_{B2}) = \frac{(4\pi)^4}{2 + 2\Delta} \begin{cases} \left[r_{A1}^2 \Psi_{100}^2(r_{A1}) r_{B2}^2 \Psi_{100}^2(r_{B2})\right] r_{A2}^2 r_{B1}^2 \\ + 2\left[r_{A1} \Psi_{100}(r_{A1}) r_{A2} \Psi_{100}(r_{A2}) r_{B1} \Psi_{100}(r_{B1}) r_{B2} \Psi_{100}(r_{B2})\right] r_{A1} r_{A2} r_{B1} r_{B2} \\ + \left[r_{A2}^2 \Psi_{100}^2(r_{A2}) r_{B1}^2 \Psi_{100}^2(r_{B1})\right] r_{A1}^2 r_{B2}^2 \end{cases} \right\}$$

#### $(r\Psi)^2$ is a measure of electron weight localization



#### D<sub>2</sub> Molecule Electron Localization: 2/2



## 3.2) D<sub>2</sub> Langevin Equation



#### Potential of "dede"-type Molecule

with  $a_0 = 0.053$  nm (Bohr radius) and  $Z = e^*/e$ .

We also solved an atomic de\* system to obtain ground state energy Vhas:

$$V_{\rm h} = -13.6Z^2/(m_{\rm c}/m^*).$$
 (3.26)

For dde\*e\* molecule state with double electrons or e\* s, we also extend the solution for ddee given in the text [45] and we have obtained screened potential function  $V_{sc^*c^*}$  as:

$$V_{sc^*c^*}(R) = 2V_h + e^2/R + (2J + J' + 2\Delta K + K')/(1 + \Delta^2).$$
(3.27)

Here the cross-Coulomb integral J' and cross exchange integral K' are given as:

$$J' = (Z^2 e^2/a)(1/y - \exp(-2y))(1/y + 11/8 + 3y/4 + y^2/6),$$
(3.28)

$$K' = (Z^2 e^2 / 5/a) [-\exp(-2y)(-25/8 + 23y/4 + 3y^2 + y^3/3) + (y/6)((0.5772 + \log y)\Delta^2 + (\Delta')^2 E_i(-4y) - 2\Delta\Delta' E_i(-2y))]$$
(3.29)

with

$$\Delta' = \exp(-y)(1 - y + y^2/3), \tag{3.30}$$

$$E_{i}(y) = -\int_{0}^{\exp(-y)} (1/\log x) \, dx.$$
(3.31)



## 3.3) D<sub>2</sub><sup>+</sup> (dde) Langevin Equation

$$m_{d} \frac{d^{2} R_{dd}}{dt^{2}} = -2 \frac{e^{2}}{R_{de}^{2}} + \frac{e^{2}}{R_{dd}^{2}} + \frac{m_{e} v_{e}^{2}}{R_{e}} - \frac{\partial V_{s}(R_{dd};1,1)}{\partial R_{dd}} + f(t)$$

$$-e^{2}\left\langle \frac{2}{R_{de}^{2}} - \frac{1}{R_{dd}^{2}} \right\rangle + \left\langle \frac{m_{e}v_{e}^{2}}{R_{e}} \right\rangle = 0$$

<R<sub>dd</sub>> = 138 pm

<R<sub>de</sub>> = 86.9 pm

<Re> = 52.9 pm

$$m_{d} \frac{d^{2} \langle R_{dd} \rangle}{dt^{2}} = -\frac{\partial V_{s}(R_{dd};1,1)}{\partial \langle R_{dd} \rangle}$$

<R<sub>dd</sub>>(∞)=R<sub>gs</sub>=138 pm <H>=-15.1eV <Electron K.E>=13.6eV





#### Potential for "dde"-type Molecule

Screened potentials  $V_{sn}(m^*/m_c, e^*/e)(R)$  were calculated for dde\* molecular states using extended solutions for dde state given in a text of quantum mechanics by the well-known technique of variational method [45] as:

$$V_{s(m^*/m_e,e^*/e)}(R) = V_{\rm h} + e^2/R + (J+K)/(1+\Delta), \tag{3.20}$$

where the Coulomb integral J, the exchange integral K, and the non-orthogonal integral  $\Delta$  are given as [45]:

$$J = Z(e^{2}/a)[-1/y + (1+1/y)\exp(-2y)],$$
(3.21)

$$K = -Z(e^2/a)(1+y)\exp(-y), \qquad (3.22)$$

$$\Delta = (1 + y + y^2/3) \exp(-y). \tag{3.23}$$

With

$$Y = R/a, \tag{3.24}$$

$$a = a_0/Z/(m^*/m_c)$$
 (3.25)

4. QM-Average for Complex D-cluster under Platonic Symmetry

• Average on Electron-wave function is replaced with Friction (Constraint) as

$$\langle Constraint \rangle_{electron-wave} = -N_f \frac{\partial V_{si}(R_{dd};1,1)}{\partial R_{dd}}$$

Nf : Number of faces for Platonic polyhedron Vsi: D<sub>2</sub> (i=2) or D<sub>2</sub><sup>+</sup> (i=1) trapping potential

Average on d-d wave function: using

$$\Psi(R,R') = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-(R'-R)^2/(2\sigma^2))$$

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## QM Average of Langevin Equation: for $N_e > 2$

$$N_e m_d \frac{d^2 R}{dt^2} = -\frac{k}{R^2} - N_f \frac{\partial V_s}{\partial R} + f(t)$$

Ne: Number of d-d edges

$$N_{e}m_{d}\left\langle\Psi(R,R')\left|\frac{d^{2}R}{dt^{2}}\right|\Psi(R,R')\right\rangle = -\left\langle\Psi(R,R')\left|\frac{k}{R^{2}}\right|\Psi(R,R')\right\rangle$$
$$-N_{f}\left\langle\Psi(R,R')\left|\frac{\partial V_{s}}{\partial R}\right|\Psi(R,R')\right\rangle + \left\langle\Psi(R,R')\left|f(t)\right|\Psi(R,R')\right\rangle$$

$$\Psi(R,R') = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-(R'-R)^2/(2\sigma^2))$$

**Gaussian Wave Function** 

$$N_{e}m_{d}\frac{d^{2} < R >}{dt^{2}} = -\frac{k}{R^{2}} - N_{f}\frac{\partial V_{s}}{\partial R} + < f(t) >$$

Equation for Expectation Value

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	N	<sub>e</sub> m a	$\frac{d^2 R}{dt^2}$	= -	$-\frac{k}{R^2}-$	N	$\frac{\partial V_s}{\partial R} +$	f(t)
				Cen Cou	tripetal lomb Force	F	riction by lectron Cloud	QM Fluctuation Of Force
-	Table-1: parameters of D-cluster Langevin equation							
	cluster		N <sub>e</sub> : Number of d-d edges		k: Total Coulomb Force parameter (keVpm)		Type of electron trapping potential on a surface	N <sub>f</sub> : number of faces
	D <sub>2</sub>		1		0		i = 2	1
	$D_2^+$		1		0		i = 1	1
	$D_3^+$		3		6.13		i = 1	6
	4D/TSC		6		11.85		i = 2	6
	6D <sup>2-</sup> /OSC		12		29.3		i = 1	24

## 4.2) Application to Tri-Atomic Molecule

3D<sup>+</sup> Ion ; Semi-classical view of particle arrangement

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## 3D<sup>+</sup> Molecule

• Coulomb Energy:

$$E_{C} = -6\frac{e^{2}}{R_{de}} + 3\frac{e^{2}}{R_{dd}} + \frac{e^{2}}{R_{ee}}$$

For Platonic arrangement:

$$E_C = -(6\sqrt{2} - 3 - \frac{\sqrt{6}}{2})\frac{e^2}{R_{dd}} = -\frac{6.13}{R_{dd}}$$

# **D**<sub>3</sub><sup>+</sup> Ion Langevin Equation



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$$3m_{d} \frac{d^{2} \langle R_{dd} \rangle}{dt^{2}} = -\frac{6.13}{\langle R_{dd} \rangle^{2}} - 6\frac{\partial V_{s}(R_{dd};1,1)}{\partial \langle R_{dd} \rangle} + \langle f(t) \rangle$$

$$\left\langle f(t) \right\rangle = \left\langle -\frac{\partial \Delta E_C}{\partial R} \mathbf{X}^2(R_{dd};\sigma,t) \right\rangle$$

:Distortion of Coulomb force from 3D Regular triangle arrangement (about 30%)

## **Summary of Known D-molecules**

- Known D-molecules are regarded as Platonic Symmetric System with orthogonal coupling of electron wave function and deuteron wave function
- Due to the Platonic symmetry, 3-dim.
   Dynamics can be treated by 1-dim.
   Dynamics using Langevin equation
- Deuteron Trapping Potential is estimated from individual Langevin equation

# 5.Now the Methodology is applied for 4D/TSC and 6D/OSC

- Formulate the central condensation force (CCF) by Coulombic interaction
- Formulate the fluctuation force term by change of CCF in deformed state from the Platonic symmetry
- Define cluster trapping potential (timedependent)
- Excute numerical calculation



## Coulomb Energy of TSC

System Coulomb Energy for CCF

$$\left\langle E_{C-TSC} \right\rangle = 12\left(-\frac{e^2}{R_{de}}\right) + 12\left(\frac{e^2}{R_{dd}}\right) + 4\left(-\frac{e^2}{\sqrt{3}R_{de}}\right) = -\frac{8.38}{R_{de}}$$

In keV unit with R in pm unit

$$R_{dd} = \sqrt{2}R_{de}$$

$$\left\langle E_{k,e-ball} \right\rangle = 4\left(\frac{1}{2}m_e v_d^2\right) = 4\left(\frac{m_e}{M_d}\right)E_d \le 0.88eV$$



#### Feature of QM Electron Cloud



b) D<sub>2</sub> molecule (stable):  $\Psi_{2D} = (2+2\Delta)^{-1/2} [\Psi_{100}(r_{A1}) \Psi_{100}(r_{B2}) + \Psi_{100}(r_{A2}) \Psi_{100}(r_{B1})] X_s(S1,S2)$ 

# Wave Function for 4D/TSC (t=0)

•  $\Psi_{4D} \sim a1 [\Psi_{100}(r_{A1}) \Psi_{100}(r_{B2}) + \Psi_{100}(r_{A2}) \Psi_{100}(r_{B1})]X_{s}(S1,S2)$  $+ a2 [\Psi_{100}(r_{A1}) \Psi_{100}(r_{D4}) + \Psi_{100}(r_{A4}) \Psi_{100}(r_{D1})]X_{s}(S1,S4)$  $+ a3 [\Psi_{100}(r_{A2}) \Psi_{100}(r_{C4}) + \Psi_{100}(r_{A4}) \Psi_{100}(r_{C2})]X_{s}(S2,S4)$  $+ a4 [\Psi_{100}(r_{B1}) \Psi_{100}(r_{D3}) + \Psi_{100}(r_{B3}) \Psi_{100}(r_{D1})]X_{s}(S1,S3)$  $+ a5 [\Psi_{100}(r_{B2}) \Psi_{100}(r_{C3}) + \Psi_{100}(r_{B3}) \Psi_{100}(r_{C2})]X_{s}(S2,S4)$  $+ a6 [\Psi_{100}(r_{C3}) \Psi_{100}(r_{D4}) + \Psi_{100}(r_{C4}) \Psi_{100}(r_{D3})]X_{s}(S3,S4)$ 

6-Bonds of "Bosonozed" electron-pairs (e↑+ e↓), which forms **Regular Tetrahedron (PA)** 

4-Electron-Centers at Vertexes of Regular Tetrahedron (PA)

 $u_{1s1}(r) = \Psi_{100}(r) = (1/\pi)^{1/2}(1/a_B)^{3/2}exp(-r/a_B)$
#### Result of Dynamic Condensation of 4D/TSC by Langevin Equation



## 5.2 4D/TSC Langevin Equation for Monte-Carlo Calculation

$$\begin{split} & 6m_d \frac{d^2 R_{dd}(t)}{dt^2} = -\frac{11.85}{[R_{dd}(t)]^2} - 6\frac{\partial V_{s2}(R_{dd}(t);1,1)}{\partial R_{dd}(t)} + \langle f(t) \rangle + f'(t) \\ & f'(t) = f(t) - \langle f(t) \rangle \\ & V_{tsc-main} = -\frac{11.85}{R_{dd}} + 6V_{s2}(R_{dd};1,1) \\ & f(t) = [-\frac{\partial \Delta E_c(R_{dd})}{\partial R_{dd}}] \operatorname{mod}[X^2(R'_{dd};R_{dd}(t))] \\ & X^2(R'_{dd};R_{dd}(t)) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-(R'_{dd} - R_{dd}(t))^2/(2\sigma^2)] \end{split}$$



## Langevin Equation for Total TSC System with Maximum-Estimated Friction



# Verlet's Method

$$G(r,t) = \frac{1.975}{m_d [R(0) - r(t)]^2} + \frac{1}{m_d} \frac{\partial V_s(R_{dd};m,Z)}{\partial R_{dd}}$$

$$R_{dd}(t) = R_0 - r(t)$$

$$\frac{d^2 r(t)}{dt^2} = G(r,t)$$

$$r(t + \Delta t) = r(t) + v(t)\Delta(t) + \frac{1}{2}G(r,t)(\Delta t)^2$$

$$v(t + \Delta t) = v(t) + \frac{\Delta t}{2}[G(r,t + \Delta t) + G(r,t)]$$



## Adiabatic Potential for Molecule dde\* and its ground state squared wave function





After Hale-Tally, Proc. ICCF4, Trans. Fusion Technology, 26,4T (1994)448



### **Distortion of Double Platonic Arrangement**



12 Attractive Coulomb forces Between d-e pairs on 6 surfaces And 4 Attractive Forces between 4 diagonal d-e pairs

6 repulsive Coulomb Forces Between electrons

6 repulsive Coulomb Forces Between deuterons



$$\begin{aligned} & \text{TSC Langevin Step2} \\ \hline 6m_d \, \frac{d^2 R_{dd}\left(t\right)}{dt^2} = -BA \times \frac{11.85}{\left[R_{dd}\left(t\right)\right]^2} - 6 \frac{\partial V_s\left(R_{dd}\left(t\right);m,Z\right)}{\partial R_{dd}\left(t\right)} + f\left(t\right) \\ & f\left(t\right) = \left[-\frac{\partial \Delta E_c\left(R_{dd}\right)}{\partial R_{dd}}\right] \text{mod}\left[X^2\left(R'_{dd};R_{dd}\left(t\right)\right)\right] \\ & \text{f(t)=0 for } R'_{dd} = \text{R}_{dd} \end{aligned}$$

$$\begin{aligned} X^2\left(R'_{dd};R_{dd}\left(t\right)\right) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\left(R'_{dd}-R_{dd}\left(t\right)\right)^2/(2\sigma^2)\right] \\ & \frac{\sigma = 0.372R_{dd}\left(t\right)}{\Delta R_{dd} = R'_{dd}-R_{dd}\left(t\right)} \end{aligned}$$

$$-\frac{\partial \Delta E_c(R'_{dd})}{\partial R_{dd}} = 6.60 \frac{\left[\Delta R_{dd}\right]^2}{\left[R_{dd}(t)\right]^4}$$

$$f(t) = f_{up}(t) + f_{down}(t)$$

Change of TSC Coulomb Energy by Distortion of Platonic Symmetry

Fluctuation of 2 d-d pairs of TSC

# Averaged Treatment of <f(t)>

$$\langle f(t) \rangle = 2 \times 6.6 \int_0^\infty \frac{[R' - R_{dd}(t)]^2}{[R_{dd}(t)]^4} X^2(R') dR'$$

$$\langle f(t) \rangle = \frac{13.2\sigma^2}{\sqrt{\pi} [R_{dd}(t)]^4} \int_0^\infty \sqrt{x} \exp(-x) dx = 13.2 \frac{\sigma^2}{[R_{dd}(t)]^4}$$

$$\sigma = 0.372 R_{dd}(t)$$

$$6m_{d} \frac{d^{2} \langle R_{dd} \rangle}{dt} = -BA \frac{11.85}{\langle R_{dd} \rangle^{2}} - 6 \frac{\partial V_{s}(R_{dd};m,Z)}{\partial \langle R_{dd} \rangle}$$

**BA = 0.846** 

## BA=0.846



Ed = 13.68 keV at Rdd = 24.97 fm, with Vtrap = -130.4 keV

# 5.3 Time Dependent dd Trapping Potential of TSC

$$6m_{d} \frac{d^{2} \langle R_{dd} \rangle}{dt^{2}} = -\frac{11.85}{\langle R_{dd} \rangle^{2}} - 6 \frac{\partial V_{s}(\langle R_{dd} \rangle; m, Z)}{\partial \langle R_{dd} \rangle} + 6.6 \left\langle \frac{(R' - R_{dd})^{2}}{R_{dd}^{4}} \right\rangle$$
Approximate TSC Trapping Potential is given as
$$V_{tsc}(R': R_{dd}(t)) = -\frac{11.85}{R_{dd}(t)} + 6V_{s}(R_{dd}(t); m, Z) + 2.2 \frac{|R' - R_{dd}(t)|^{3}}{[R_{dd}(t)]^{4}}$$

### Mean Particle Kinetic Energies of the "dede" System of TSC



#### Orbit of Electron Center: a) D2 Molecule, b) TSC



Fig.4: Time dependent behavior of effective electron wave length, a) D2 molecule, b) "d-e-d-e" EQPET molecule of 4D/TSC



Fig.6: Time variation of mean electron kinetic energy (EKE) and its wave length (EWL) during the 4D/TSC condensation motion in 1.4007fs condensation time.





- a) Mean rotation time of electron in "d-e-d-e" of TSC, mean rotation number is about 6 at every Rdd step
- b) Feature of spiral motion of electron in 1.4007 fs condensation time interval

Fig.7: Mean rotation time of electron cloud center under 4D/TSC condensation motion (left) and expanded feature of electron spiral motion (right)





- a) Mean rotation time of electron in "d-e-d-e" of TSC, mean rotation number is about 6 at every Rdd step
- b) Feature of spiral motion of electron in 1.4007 fs condensation time interval

Fig.7: Mean rotation time of electron cloud center under 4D/TSC condensation motion (left) and expanded feature of electron spiral motion (right)

## 5.4 Application to 6D/OSC





## Langevin Equation for 6D(2-)/OSC







# 6. HMEQPET Method for Fusion Rate Quantification

 The role and merit of HMEQPET (heavy mass electronic quasi-particle expansion theory) method for approximating time-dependent TSC trapping potential and relating to the estimation of time-dependent Coulomb barrier penetration probabilities of 4d cluster is explained. HMEQPET provides a practical method for calculating time-dependent (hence timeaveraged) fusion rate under TSC condensation, based on the Fermi's first golden rule.



Table-3: Calculated HMEQPET potentials and their parameters,Egs-Vs-min gives mean relative kinetic energy of trapped d-d pair

Molecule	b0 (pm)	Rmin (pm)	Vs-min (keV)	Ed-d (keV)	Rgs (pm)	Egs (keV)
<b>D</b> 2	22	70	-0.03782	0.00268	76.69	-0.03514
dde*(2,2)	4.5	19.3	-0.1804	0.01013	21.82	-0.17027
dde*(5,2)	1.9	7.6	-0.4509	0.0208	8.72	-0.43007
dde*(10,2)	0.90	3.8	-0.9019	0.0418	4.36	-0.86012
dde*(20,2)	0.45	1.9	-1.8039	0.0837	2.18	-1.7202
dde*(50,2)	0.18	0.76	-4.5097	0.2094	0.873	-4.3003
dde*(100,2)	0.09	0.38	-9.0194	0.4196	0.436	-8.5998
dde*(200,2)	0.045	0.19	-18.039	0.843	0.218	-17.196
dde*(500,2)	0.018	0.076	-45.097	2.135	0.0873	-42.968
dde*(1000,2)	0.009	0.038	-90.194	4.336	0.0436	-85.858
dde*(2000,2)	0.0045	0.019	-180.39	8.984	0.0218	-171.406

Due to HUP, relative d-d kinetic energy should go up finally to about 10keV.

## HMEQPET Method

- Time-dependent (Rdd-dependent) d-d trapping potential of TSC can be approximated by Vs(R;m,2) potential for dde\*(m,2) EQPET molecule.
- Heavy Mass Cooper Pair Concept: e\*(m,2)
- We got empirical relations:

$$b_0(m,2) = 0.206R_{gs}(m,2)$$

$$m = 9000 / b_0(m,2)$$

### Adiabatic Potential for Molecule dde\* and its ground state squared wave function



### Barrier Factor by Heavy Mass EQPET (HMEQPET)

$$b_0(m,2) = 0.206R_{gs}(m,2)$$
  $m = 9000 / b_0(m,2)$ 

$$\Gamma_{dd}(m,Z) = 0.218 \sqrt{\mu} \int_{r_0}^{b_0(m,Z)} \sqrt{V_s(R_{dd};m,Z) - E_d} dR_{dd}$$

$$P_{nd}(m,Z) = \exp(-n\Gamma_{dd}(m,Z))$$

Instead of biasing Vs potential with –Vs-min, we regard that Γdd for Rgs=b0 is approximate solution.

Table-2: Calculated time-dependent (equivalently  $R_{dd}$  dependent) barrier factors of 4D/TSC condensation motion

Elapsed Time (fs)	R <sub>dd</sub> (pm)	P <sub>2d</sub> : 2D barrier facotor	P <sub>4d</sub> : 4D barrier factor
0	74.1 (D <sub>2</sub> molecule)	1.00E-85	1.00E-170
1.259	21.8 (dde*(2,2); Cooper pair	1.30E-46	1.69E-92
1.342	10.3	2.16E-32	4.67E-64
1.3805	4.12	9.38E-21	8.79E-41
1.3920	2.06	6.89E-15	4.75E-29
1.3970	1.03	9.69E-11	9.40E-21
1.39805	0.805 (muon-dd molecule)	1.00E-9	1.00E-18
1.39960	0.412	9.40E-7	2.16E-13
1.40027	0.206	3.35E-5	1.12E-9
1.40047	0.103	1.43E-3	2.05E-6
1.40062	0.0412	1.05E-2	1.12E-4
1.40070	0.0206 (TSC-min)	4.44E-2	1.98E-3

## 7.1. Fusion Rate for Steady dde\* molecule

• <Fusion Rate per pair> =  $T_n |\Psi(r0)|^2$ 

 $T_n = (4\pi/h) < \Psi_f | W(R) | \Psi_i > / < \Psi_f | \Psi_i >$ W(R) : imaginary part of nuclear optical potential Hint = U(R) = V(R) + iW(R) |  $\Psi(r0) |^2$  : (Coulomb barrier penetration probability at R=r0) R: d-d distance

### Fusion Rates of Steady State dde\* Molecules:

$$\left|\lambda_{nd}\right| = \frac{2}{\hbar} \langle W \rangle P_{nd}\left(r_{0}\right) = 3.04 \times 10^{21} P_{nd}\left(r_{0}\right) \langle W \rangle$$

Regarding bo as R<sub>gs</sub>, we get P<sub>nd</sub>(r<sub>0</sub>) values.

Here ro is 5 fm.

Molecule	R <sub>dd</sub> =R <sub>gs</sub>	$P_{nd}(r_0);$	<w></w>	$\lambda$ 2d	$\lambda$ 4d
	(pm)	Barrier-	(MeV)	(f/s)	(f/s)
		Factor			
$D_2$	74.1	1.0E-85	0.008	2.4E-66	
dde*(2,2)	21.8	1.3E-46	0.008	3.2E-27	
$\mu$ dd	0.805	1.0E-9	0.008	2.4E+10	
4D/TSC-min	0.021	1.9E-3	62		3.7E+20

4D/TSC-min exists within  $\Delta t=2x10^{-20}$  s at final stage of condensation: Decay of TSC: exp(-  $\lambda$  4d  $\Delta t$ )= exp(-7.6)=0.0006 $\rightarrow$  4D fusion by 100% per TSC Generation. 4D Fusion Rate (1/s) becomes 4D/TSC Production Rate (1/s).

# <W> value Estimation

• Using  $T_n \sim (PEF)^5$  in S-value analysis:

Cluster	<w> (MeV)</w>
DD	0.008
DT	0.115
3D	1.93
4D	62.0

## Scaling of PEF (Pion Exchange Force) for Nuclear Fusion by Strong Interaction

Two Body Interaction:	PEF = 1
$n + \pi^+ \rightarrow p$	
(udd) (u <mark>d</mark> *) (uud)	:u;up quark
$p + \pi^- \rightarrow n$	:d;down quark
(uud) ( <mark>u*</mark> d) (udd)	: <mark>u*</mark> ; anti-up quark
	: d* ; anti-down quark

For D + D Fusion; PEF = 2



## One Pion Exchange Potential and PEF

One Pion Exchange Potential (Hamada-Johnston Potential)

$$V_{OPEP}(x) = v_0 \cdot (\vec{\tau}_1 \cdot \vec{\tau}_2) \left\{ \vec{\sigma}_1 \cdot \vec{\sigma}_2 + (1 + \frac{3}{x} + \frac{3}{x^2}) S_{12} \right\} \frac{\exp(-x)}{x}$$

$$x = \frac{m_{\pi}c}{\hbar}r = \frac{r}{1.43}[fm] \qquad \text{Yukawa Potential} \qquad Y(x) = \frac{\exp(-x)}{x}$$

$$v_0 = \frac{1}{3} \frac{f^2 m_{\pi} c^2}{\hbar c} = 3.65 [MeV] \quad S_{12} = 3 \frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

$$\langle OnePEF \rangle = -\frac{\partial \langle V_{OPEP}(x) \rangle_{\tau,\sigma}}{\partial r} = -\frac{1}{1.43} \frac{\partial \langle V_{OPEP}(x) \rangle_{\tau,\sigma}}{\partial x}$$

### D-D Fusion: Strong Force vs. Coulomb Force


# **Estimation of S-value**

- Scaling by PEF-values:
  - U(r) = V(r) + iW(r)

 $W(r) \sim W_0 \delta(r - r0)$ 

- PEF reflects size of contact sticking surface for fusion reaction by charged pion exchange: Sn(0) ~ Tn<sup>2</sup> ~ (PEF)<sup>N</sup>
- Sdd=1.1E2 keVb, Sdt = 2E4 keVb, with PEFdd =2, PEFdt=3, PEF4d=12
- N is roughly 11.4 to give S<sub>4d</sub> = 1E11 keVb

#### Extrapolation of S(0) to multi-body D-fusion



# 7.2. 4D Fusion and <sup>4</sup>He Production Rate by TSC (Time-Dependent Fusion Rate)

- t<sub>c</sub> : Condensation Time of TSC (1.4007 fs)
- $\eta_{4d}$ : 4D Fusion Yield per TSC  $\eta_{4d} = 1 - \exp(-\int_0^{t_c} \lambda_{4d}(t) dt)$

$$\lambda_{4d}(t) = 3.04 \times 10^{21} \langle W \rangle P_{4d}(r_0; R_{dd}(t)) = 1.88 \times 10^{23} P_{4d}(r_0; R_{dd}(t))$$

$$\int_{0}^{t_{c}} \lambda_{4d}(t) dt = 1.88 \times 10^{23} \int_{0}^{t_{c}} P_{4d}(r_{0}; R_{dd}(t)) dt \qquad \int_{0}^{t_{c}} P_{4d}(r_{0}; R_{dd}(t)) dt = 2.31 \times 10^{-22}$$

$$Y_{4d} = Q_{tsc} \eta_{4d}$$
Macroscopic 4D Fusion Production Rate $\eta_{4d} \cong 1.0$  $Y_{4d} \approx Q_{tsc}$ Qtsc : TSC Generation Rate

### 8. Decay-Channel of <sup>8</sup>Be for S-Wave

- $4D \rightarrow {}^{8}Be(0+; 47.6 \text{ MeV})$  :
- $^{8}Be(0+) \rightarrow ^{4}He(0+) + ^{4}He(0+) + 91.86 \text{ keV}$

### Others (below) are forbidden by Spin-Parity Conservation (Odd parity)

- <sup>3</sup>He (1/2+)+ <sup>5</sup>He(3/2-)(n+<sup>4</sup>He) 11.13 MeV
- t (1/2+)+ <sup>5</sup>Li(3/2-)(p+<sup>4</sup>He) 21.68MeV
- p (1/2+)+ <sup>7</sup>Li (3/2-) 17.26 MeV
- n(1/2+) + <sup>7</sup>Be(3/2-) 18.90 MeV

# Initial Spin Combination of 4d/TSC; S-Wave: Only 4d(0+) makes fusion

**Entrance Channel** 

Out-going Channel

- ↑↑↑↑ ; J<sup>π</sup>=4+, T=0 (2 cases)
- ↑↑↑↓ ; J<sup>π</sup>= 2+, T=0 (8 cases)
- ↑↓↑↓ ; J<sup>π</sup>= 0+, T=0 (6 cases)
- Other cases: J<sup>π</sup>= 3-, 1 for total 4d spin

Deuteron :  $J^{\pi}$ = 1+

- <sup>8</sup>Be\*(4+: 47.6MeV) to 2<sup>4</sup>He(0+:gs); forbidden
- <sup>8</sup>Be(2+:47.6MeV) to
  <sup>4</sup>He(0+: 20.21 MeV) +
  <sup>4</sup>He(2+: 27.42MeV) 0.03MeV; forbidden
- <sup>8</sup>Be(0+:47.6MeV) to 2<sup>4</sup>He(0+:gs)+47.6MeV is allowed. (37.5%?)

#### Discussion on 2D Fusion Rate

- T<sub>(2,2)</sub> : Life Time of dde\*(2,2)
- $\eta_{2d}$ : Fusion Yield per dd pair

$$|\eta_{2d} = 1 - \exp(-\lambda_{2d(2,2)}\tau_{(2,2)})|$$

 $Y_{2d} = Q_{dde^{*}(2,2)} \eta_{2d}$ 

$$\eta_{2d} \approx \lambda_{2d(2,2)} \tau_{(2,2)}$$

a) If T(2,2) is 10<sup>4</sup> s (as X. Z. Li asserts), η<sub>2d</sub>=3.1X10<sup>-23</sup>

Assuming  $Qdde^*=10^{22}$  (1/s/cc),  $Y_{2d} = 0.3$  (f/s/cc)

b) 2D Fusion rate may be larger, when TSC under condensation would break up to two dde\* diminished size molecules. We need Monte-Carlo Langevin cal.

#### $d + d + E_k = {}^{4}He^{*}(E_x) = {}^{4}He^{*}(Q + E_k)$



D. Tilley, H. Weller, G. Hale: Nucl. Phys. A541, (1992)1-104 (Page 15)

Nestled among a series of four negative-parity, T = 1 levels in the range  $E_x = 23 - 26$  MeV (which were at least 3 MeV higher in (1973FI04)) is a new  $1^-, T = 0$  level at  $E_x = 24.25$  MeV that has important effects on the d + d reactions at low energies. Isospin mixing between this state and the  ${}^{3}P_{1}, T = 1$  level at  $E_x = 23.64$  MeV causes significant differences in the p-wave part of the d + d reactions, as have been observed in muon-catalyzed (1984BA1W) and polarized (1981AD07) d + d fusion experiments. The  $1^-$ , T = 0 level was seen by (1981GR16) in their  ${}^{2}H(d, p){}^{3}H$  analyzing-power data, but no evidence of their proposed  $4^+$  level at  $E_x = 24.6$  MeV was found by (1989HA2A) in fitting their measurements.

### $4D \rightarrow {}^{4}He + {}^{4}He + 47.6MeV$ (Final State Interaction)



### Final Sate Interaction of <sup>8</sup>Be\*(Ex=47.6MeV)

# Summary-1

- Platonic Symmetric Arrangement realizes Energy-Minimum State of Many-Body System.
- PA appears in D-atom, D<sub>2</sub>, D<sub>2</sub><sup>+</sup>,D<sub>3</sub><sup>+</sup>, and 4D/TSC.
- PA appears in CMNS of 4D/TSC for Coulombic Interaction and Strong Interaction.
- Dynamic PA is of key for 4D Cluster Fusion.
- Good solution by Molecular Dynamics with Langevin Eq., for Platonic Systems as, D, D<sub>2</sub>, D<sub>3</sub><sup>+</sup> and 4D(H)/TSC.
- About 100% 4D-Fusion per TSC generation!

# Summary 2

- Only 4D(H)/TSC can condense ultimately to 10-20 fm radius size.
- Bosonized e(1/2)+e(-1/2) coupling for dede system makes D<sub>2</sub> type faces of TSC to help ultimate condensation.
- 6D<sup>2-</sup>/OSC converges its condensation at about Rdd=40 pm, but closer d-d distance in transient.
- Single <e<sup>-</sup> >-center states for dde (D<sub>2</sub><sup>+</sup>) faces of OSC enhances constraint (friction) for condensation.

### 9. Conclusions

ACS09

- One dimensional Langevin equations for treating dynamic motion of D-clusters under Platonic symmetry were formulated.
- Only 4D/TSC makes ultimate condensation to form 10-20 fm size charge-neutral entity, among D<sub>2</sub>, D<sub>3</sub><sup>+</sup>, 4D/TSC and 6D<sup>2-</sup>/OSC.
- Almost 100% (Smaller by spin) 4D fusion with two <sup>4</sup>He ashes may take place by one 4D/TSC generation in metal-D system dynamics.