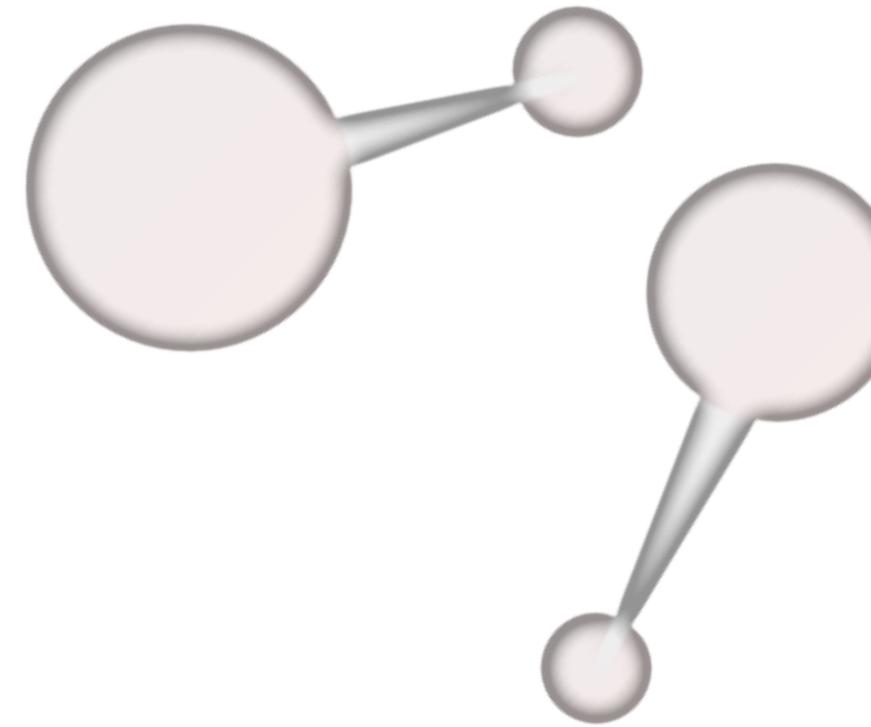


Quantum correlations *in molecular rotor systems*

QAMTS 2017

Quantum Atomic & Molecular Tunneling in Solids and Other Condensed Phases

Thomas Halverson | University of Waterloo | Waterloo ON CA

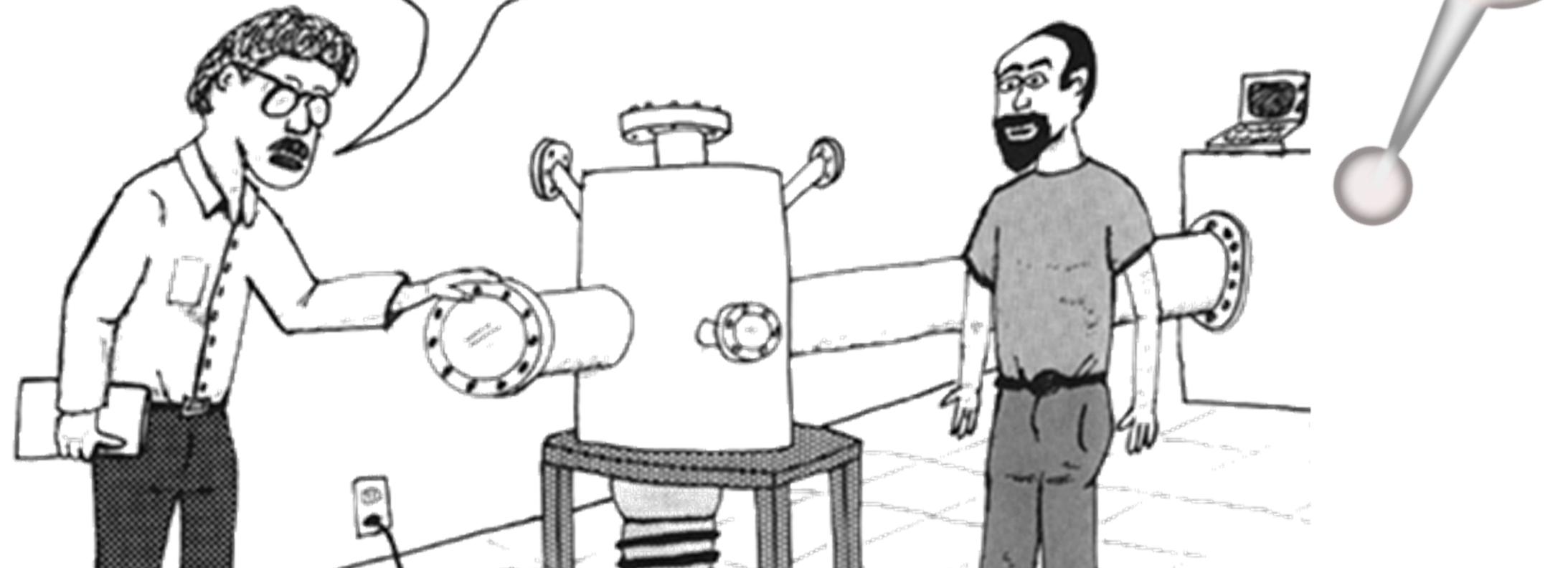


The Goal

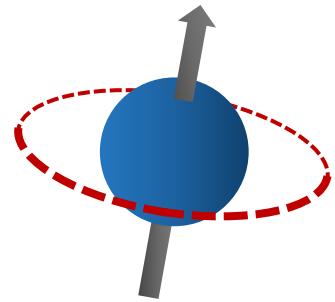


D:wave 2X™

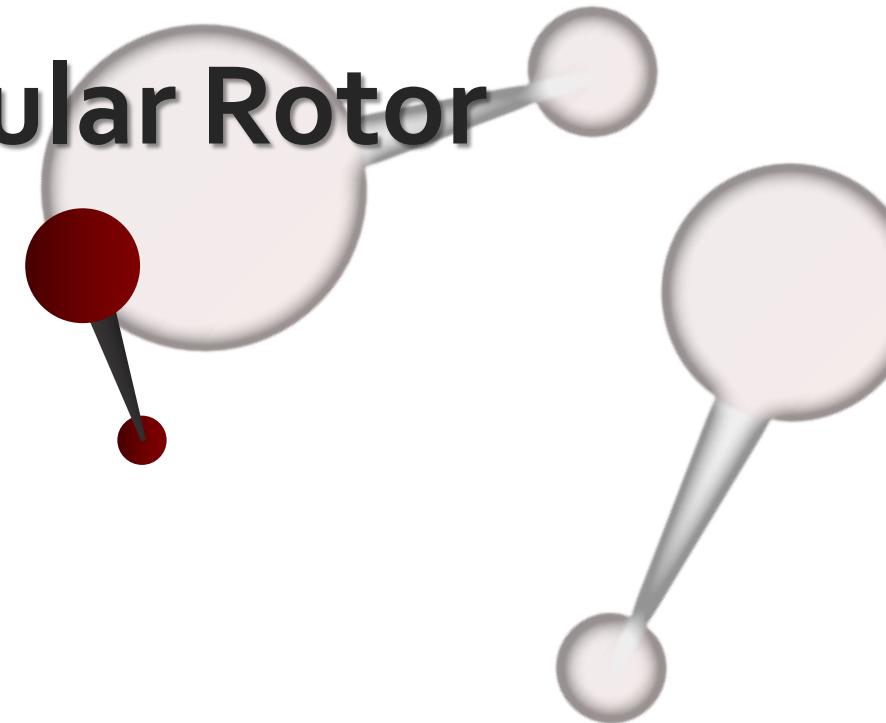
WE'VE SHOWN THAT THE RECENT UNEXPLAINED BEHAVIOR IS DIFFERENT THAN THE PREVIOUS UNEXPLAINED BEHAVIOR.



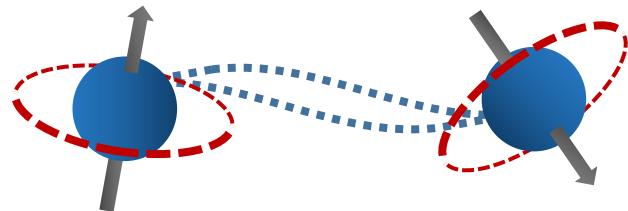
Quantum Spin



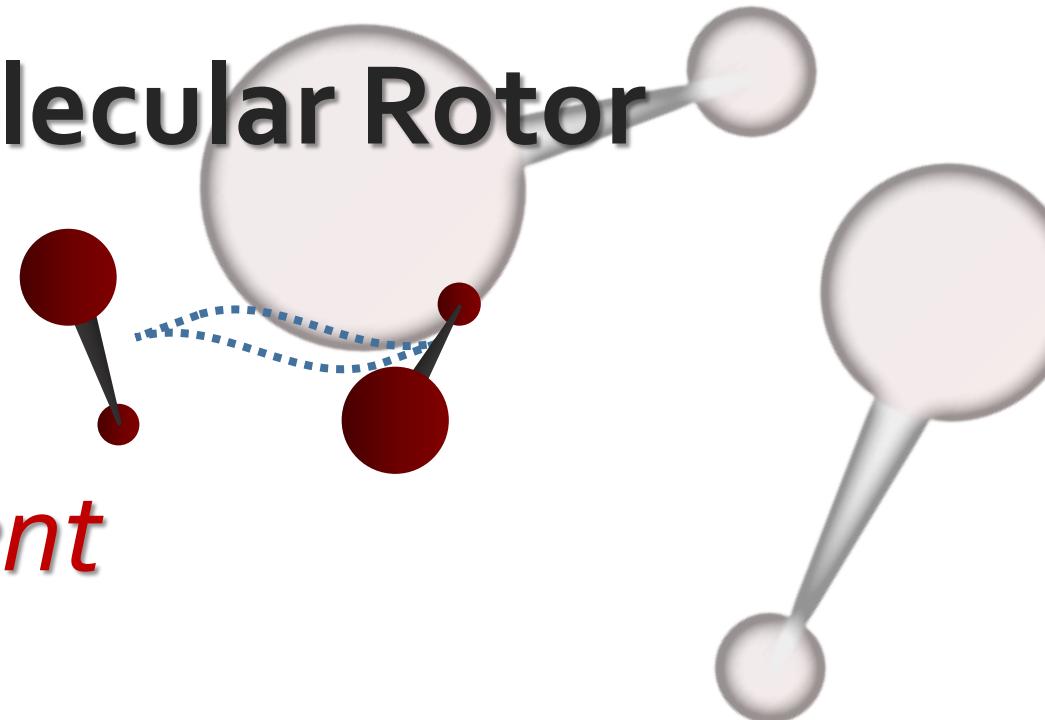
Molecular Rotor



Quantum Spin

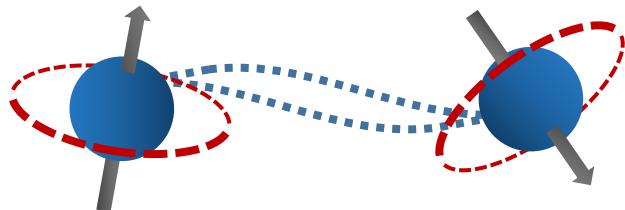


Molecular Rotor



Entanglement

Quantum Spin

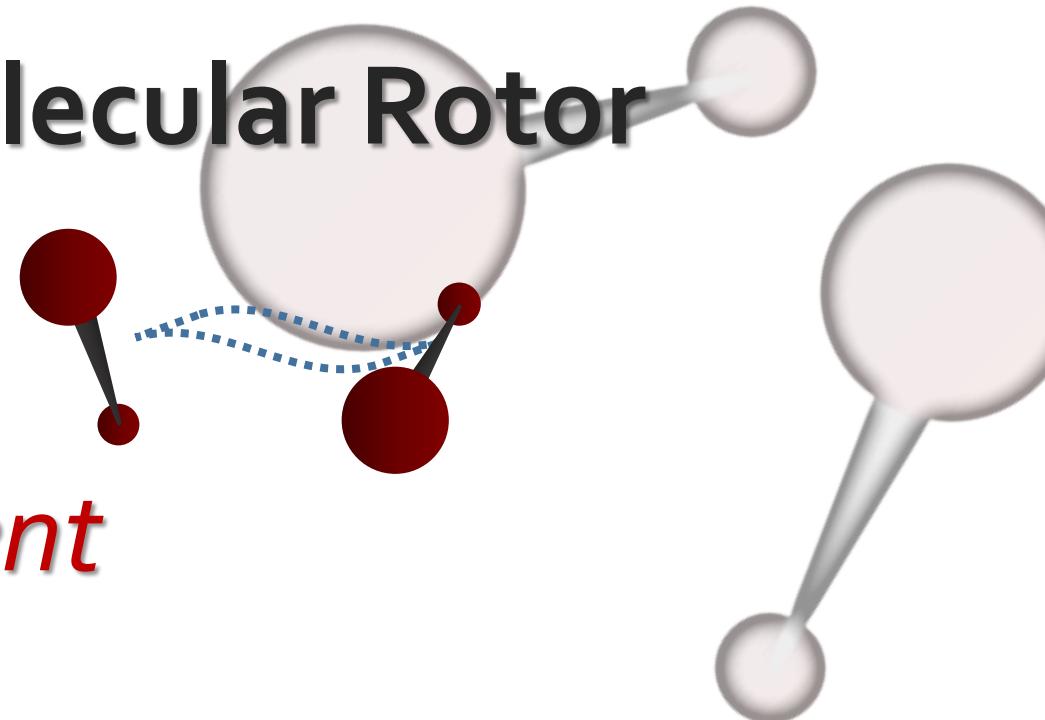


Entanglement

Bell Pair State

$$|\varphi\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$$

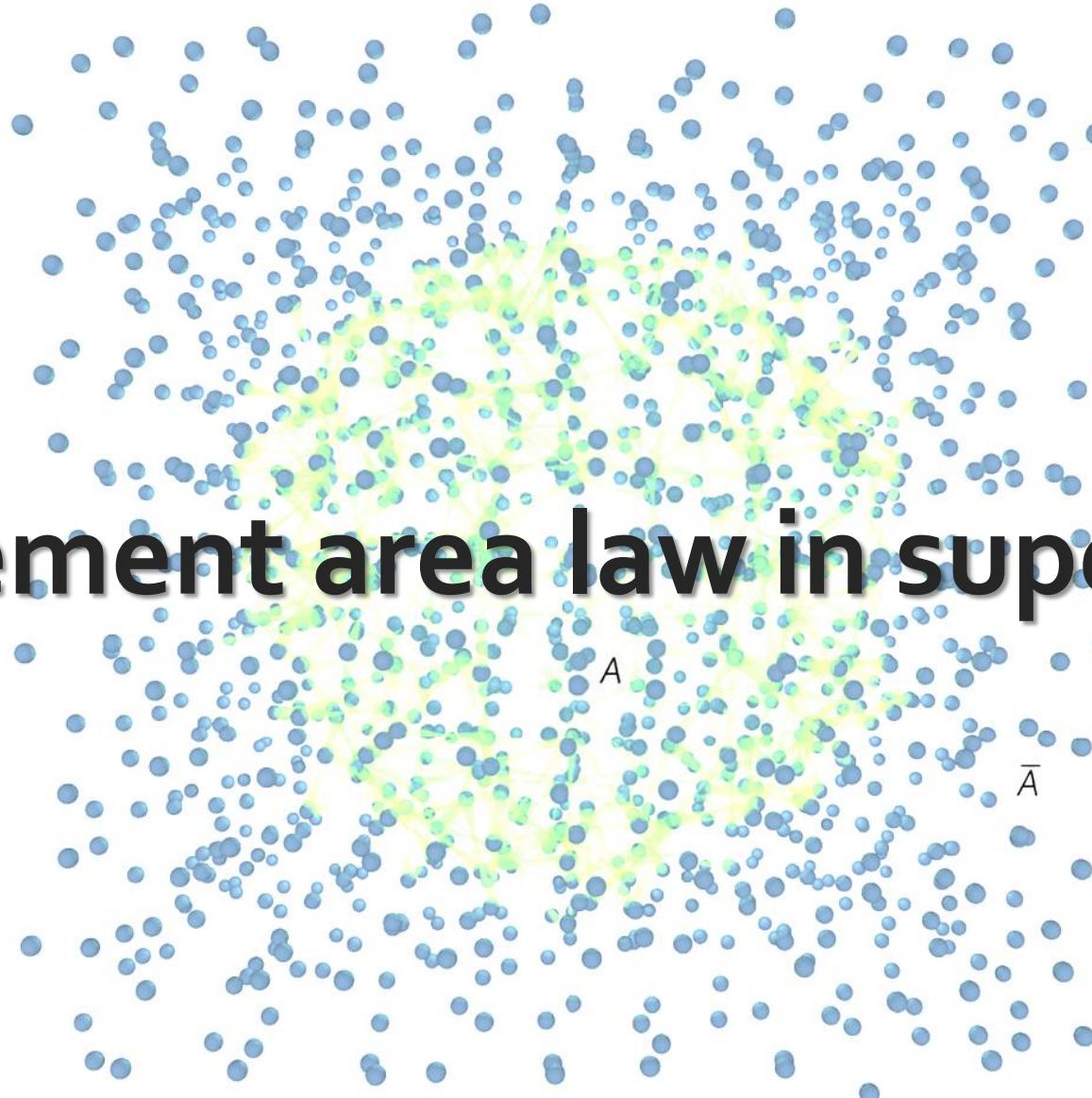
Molecular Rotor



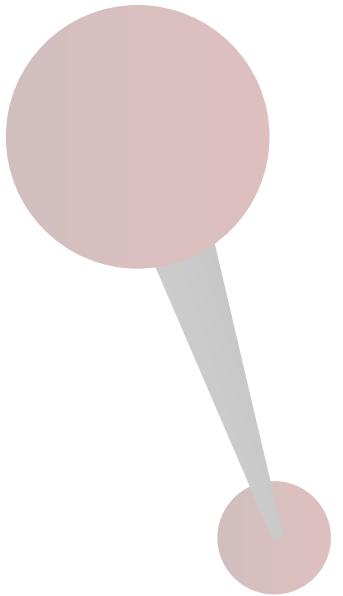
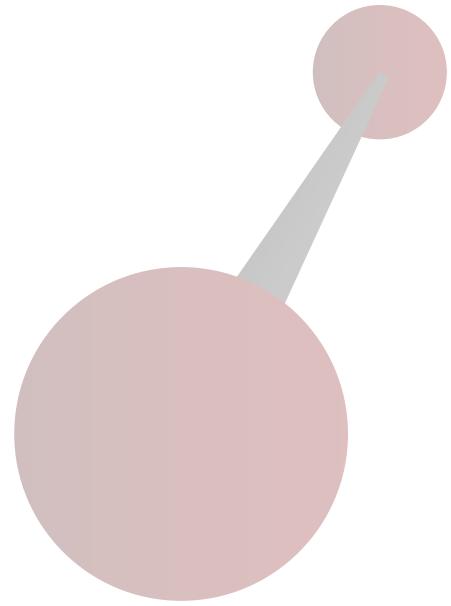
_____ Pair State

$$|\varphi\rangle = \frac{??+??}{\sqrt{2}}$$

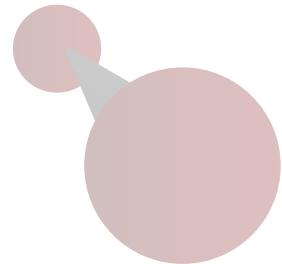
Entanglement area law in superfluid ^4He

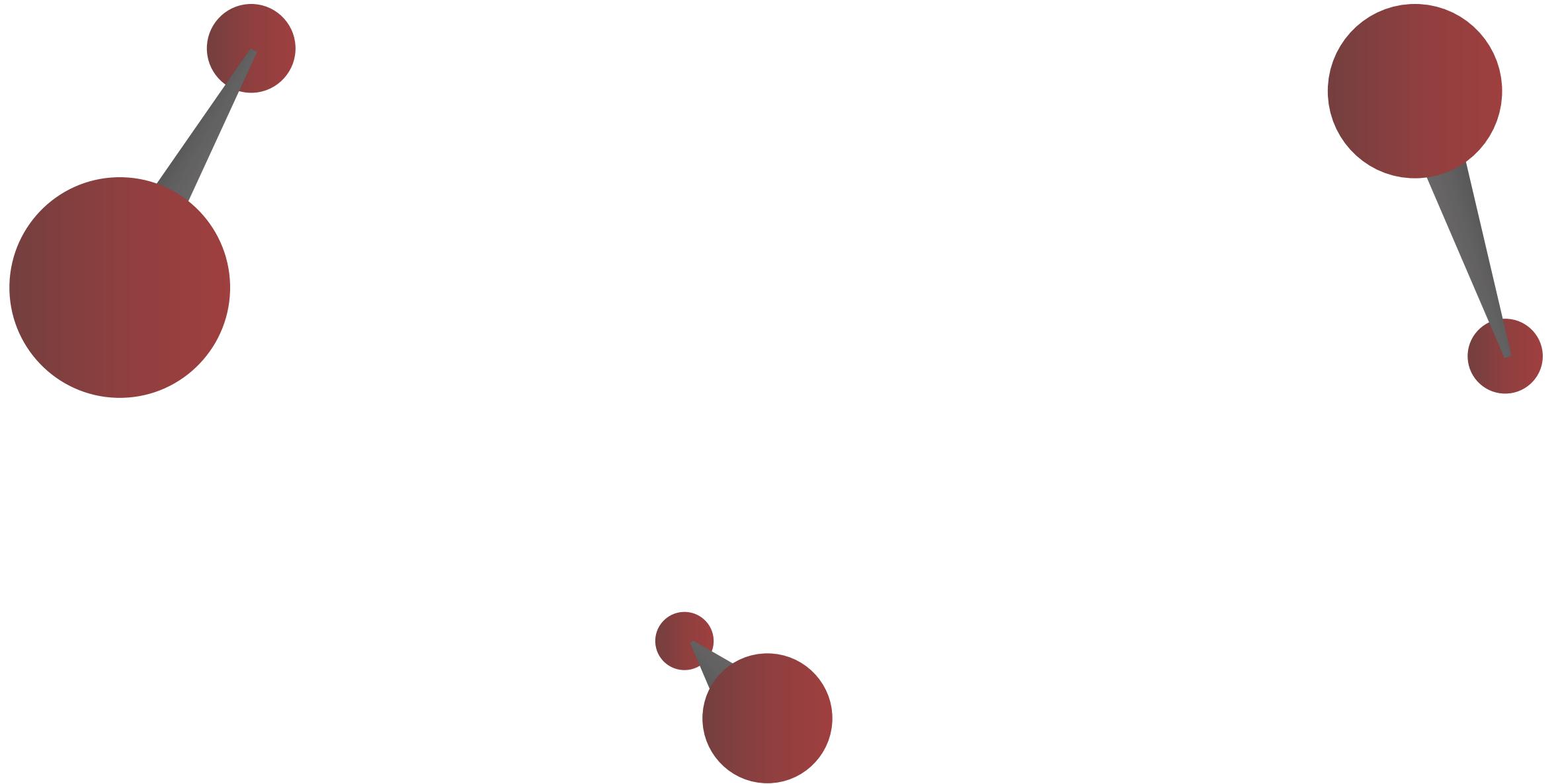


C. M. Herdman, P.-N. Roy, R. G. Melko, and A. Del Maestro, Nature Physics, 1745-2481 (2017)



para-H₂ trimer





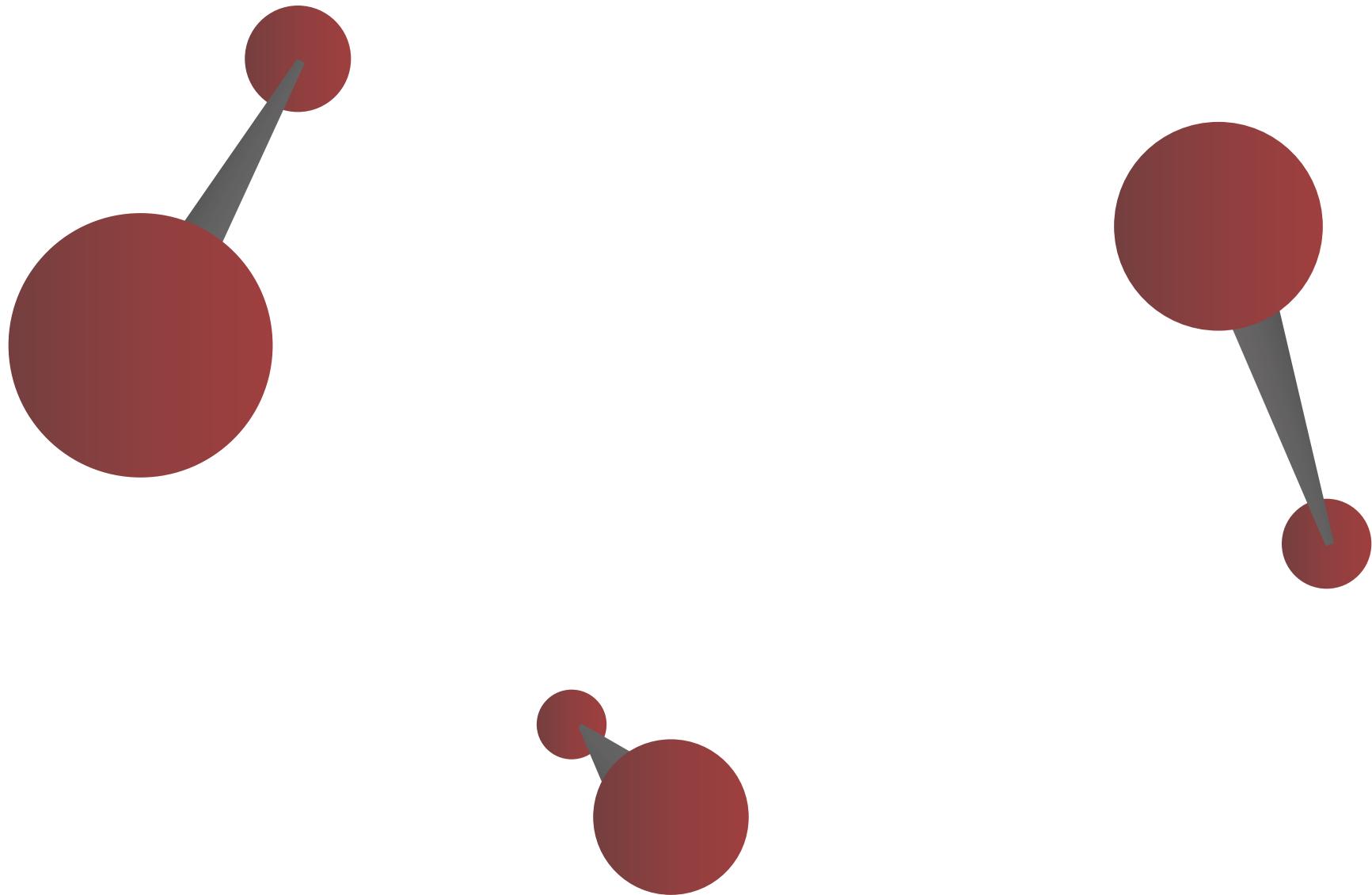
Conclusions

Confined Water

Dipole Chains

Hydrogen Clusters

Overview



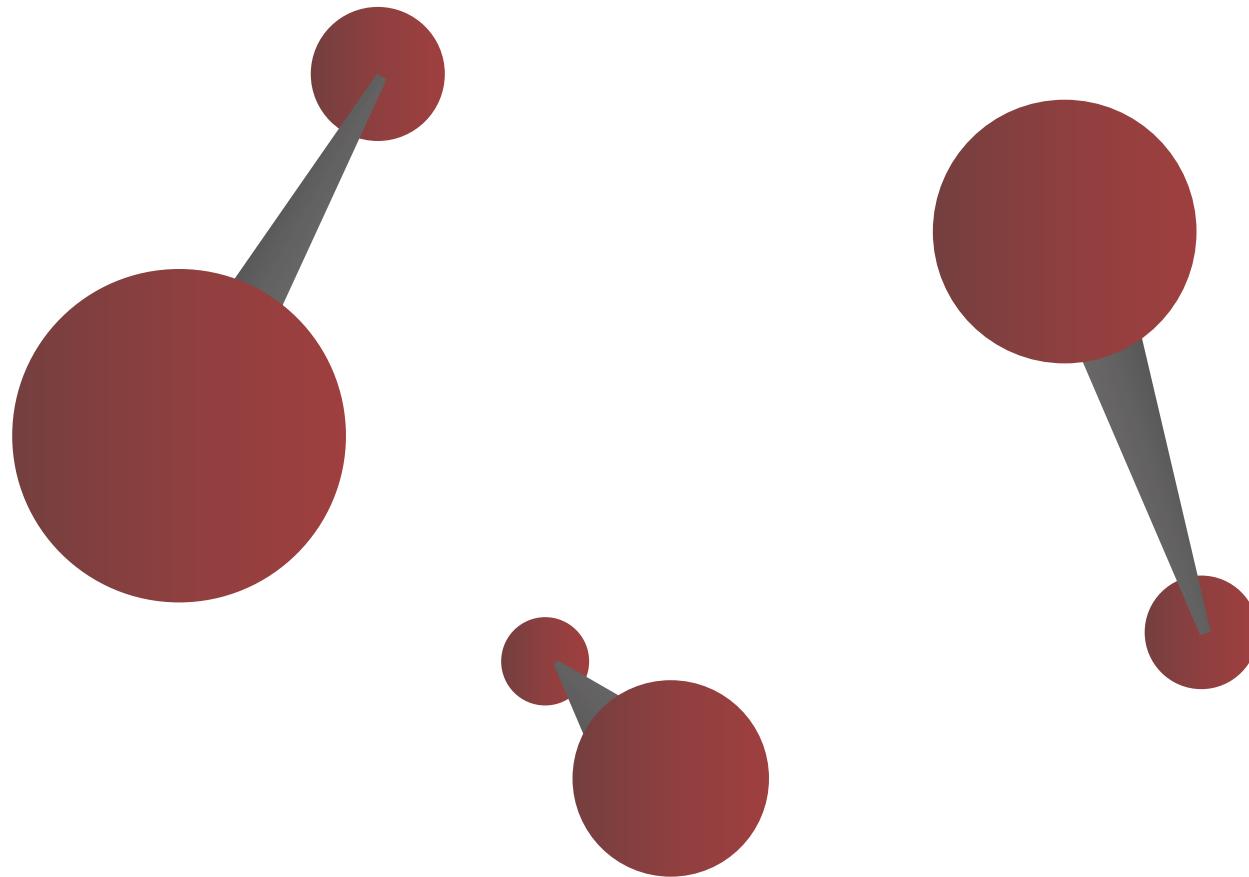
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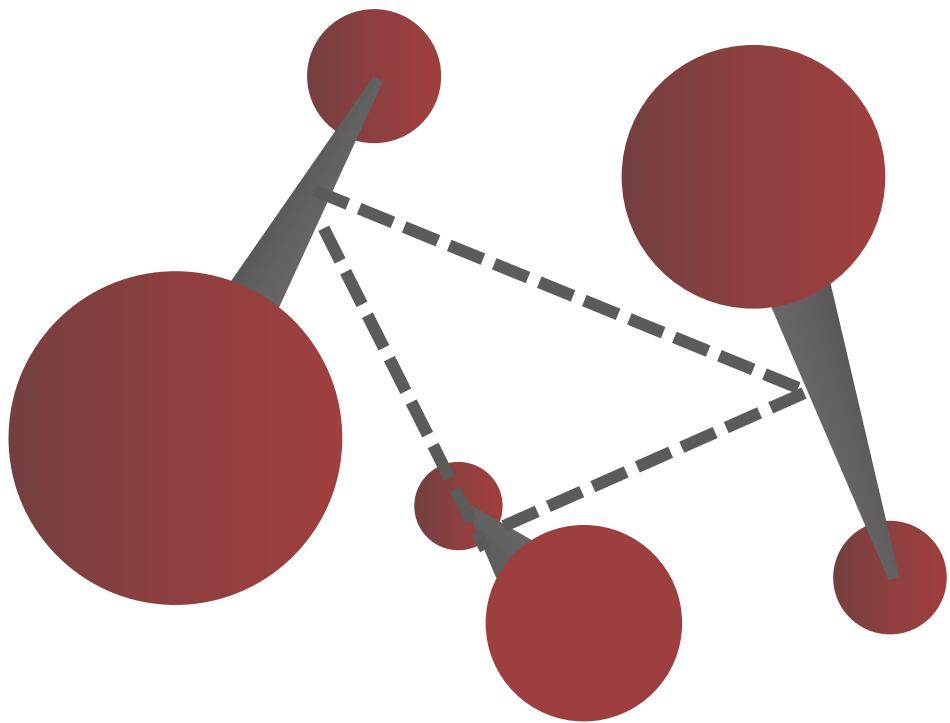
Conclusions

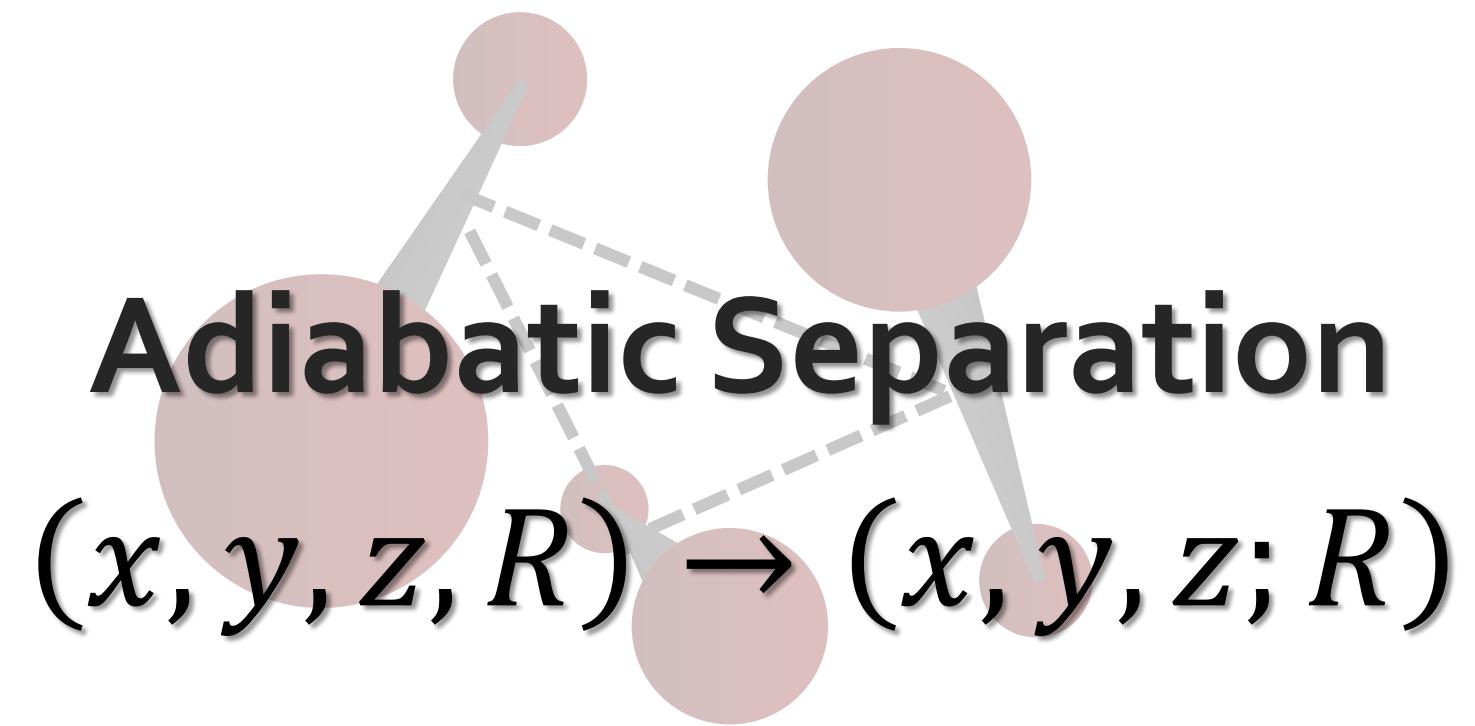
Confined Water

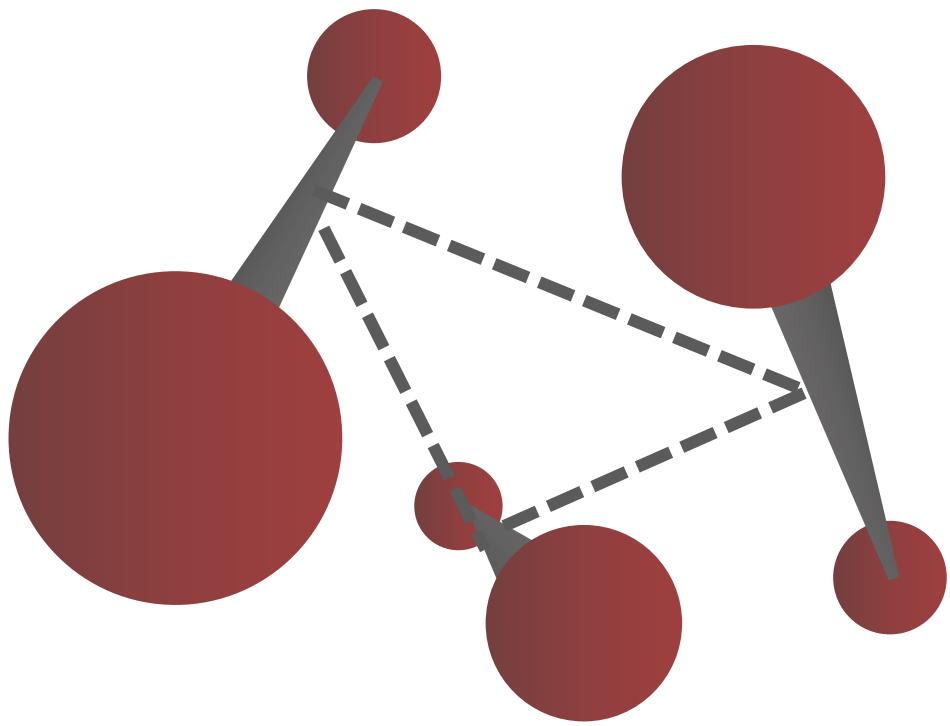
Dipole Chains

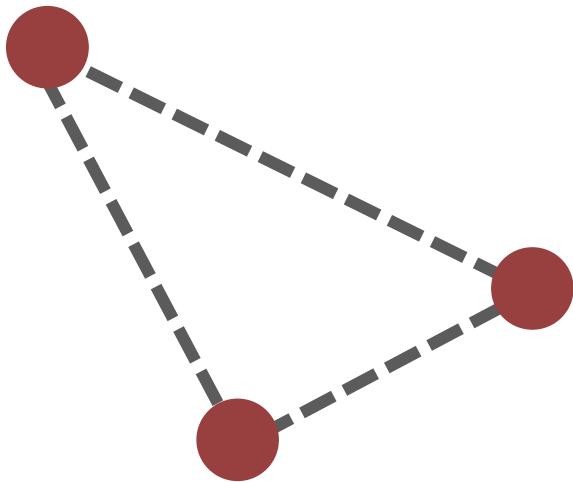
Hydrogen Clusters

Overview



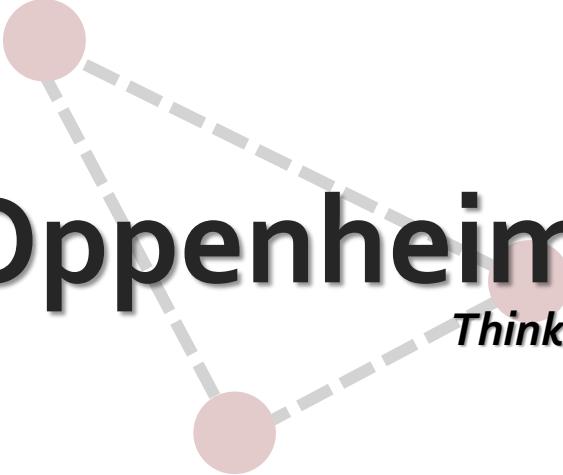








Hindered Trimer

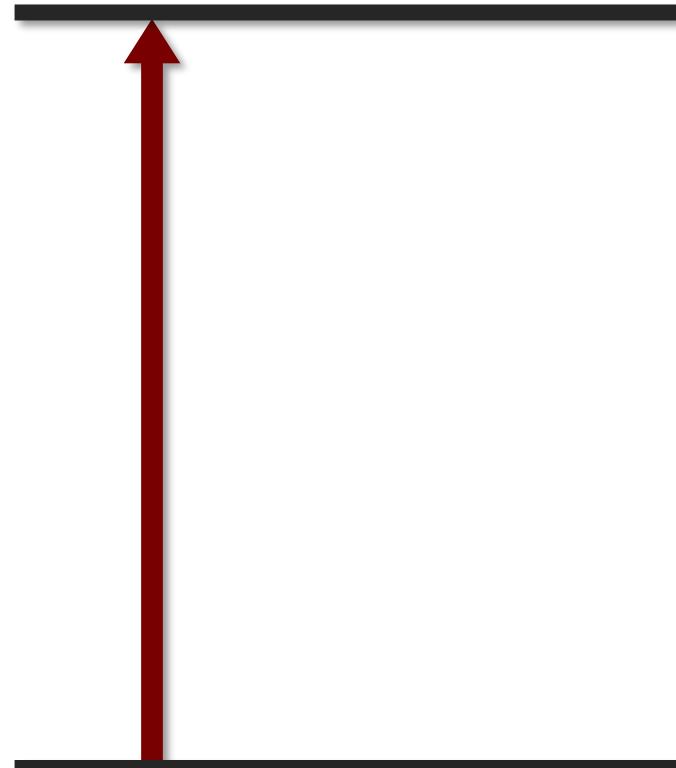


Born-Oppenheimer-Like

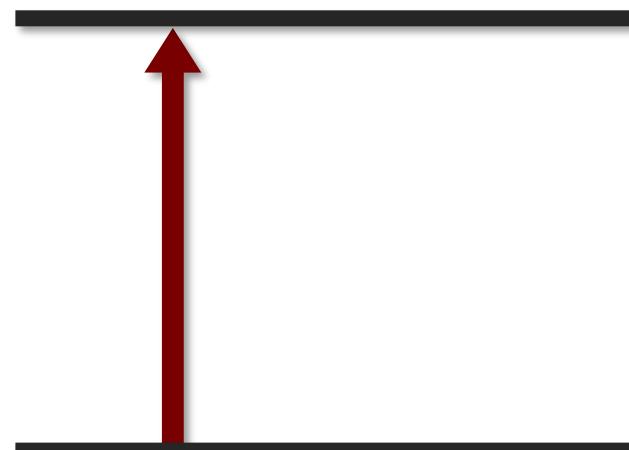
Think: Electronic Structure



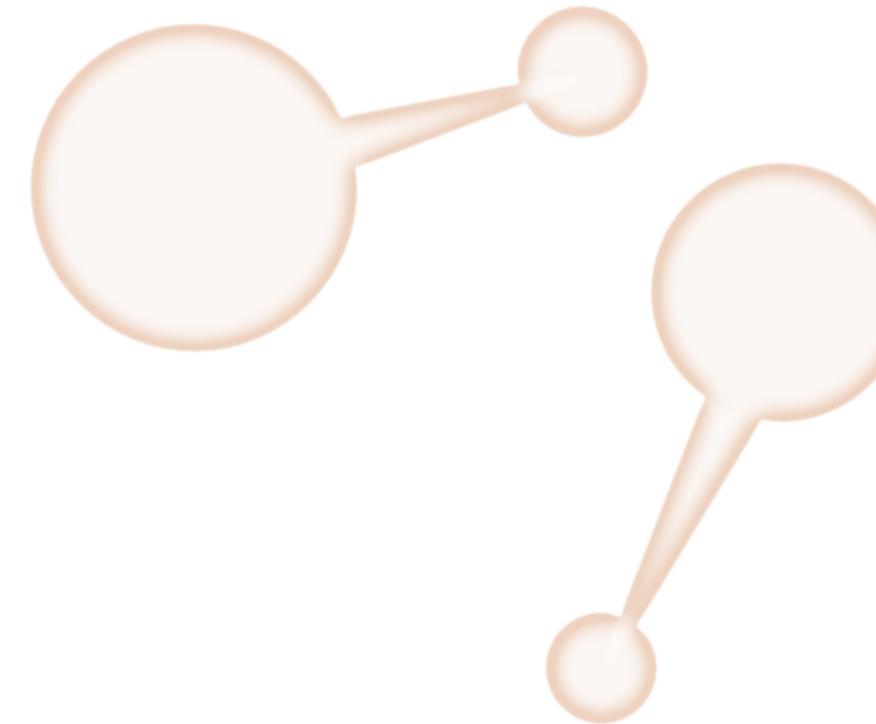
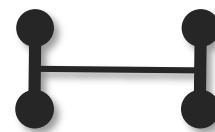
Different Energy Scales



Internal Vibration

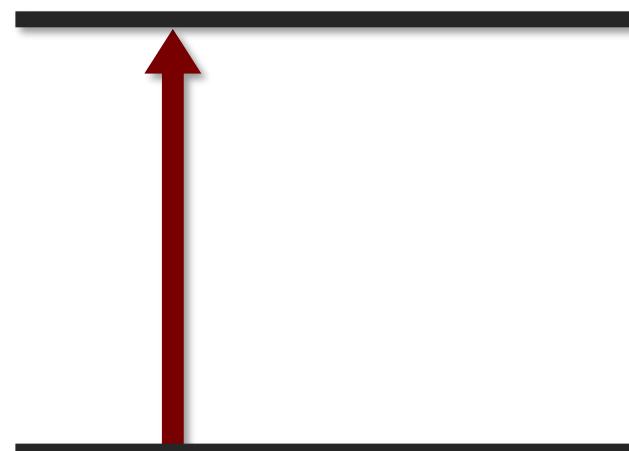
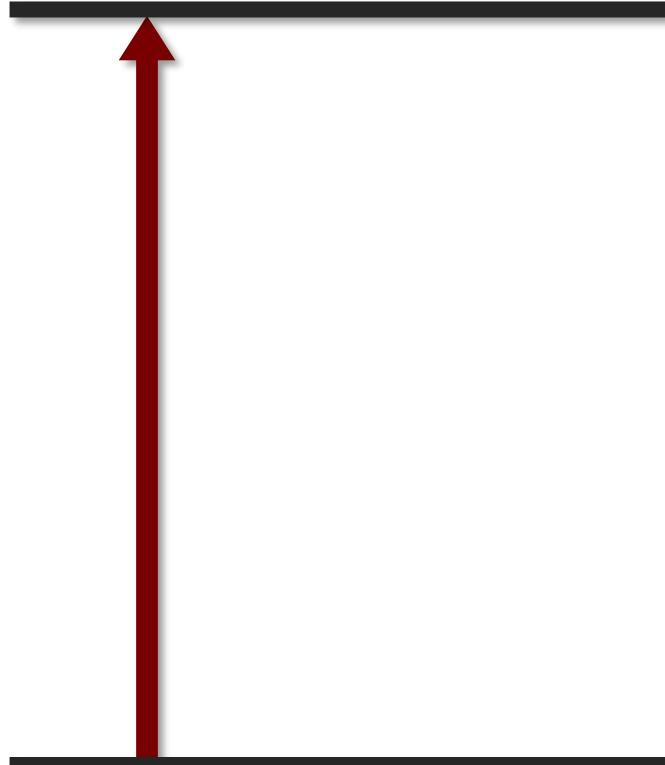


Pinned Rotation



External Vibration

$$\Delta E \approx 4000 \text{ cm}^{-1}$$

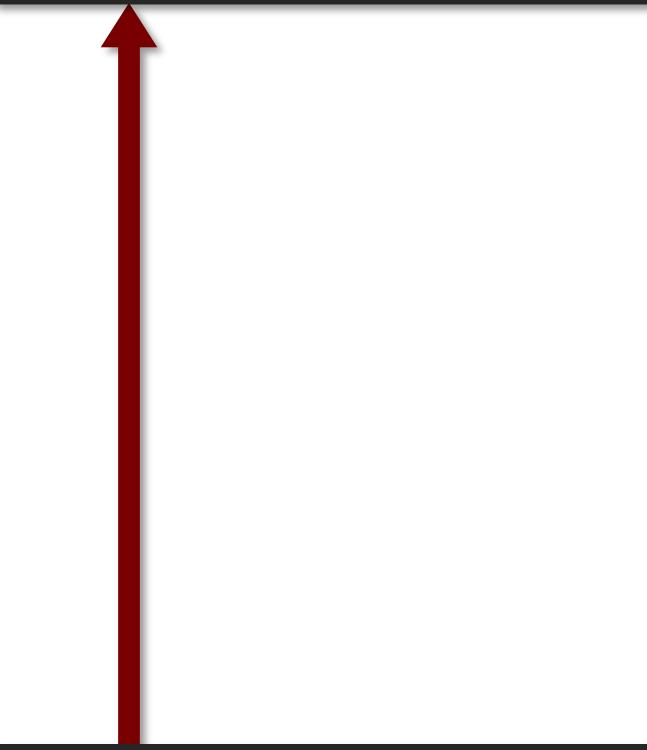


Internal Vibration

Pinned Rotation

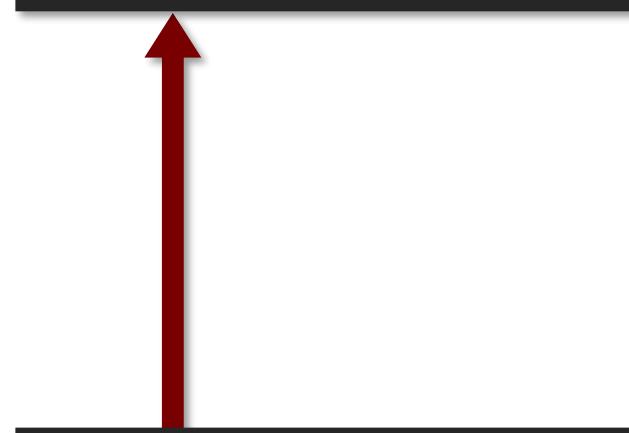
External Vibration

$$\Delta E \approx 4000 \text{ cm}^{-1}$$

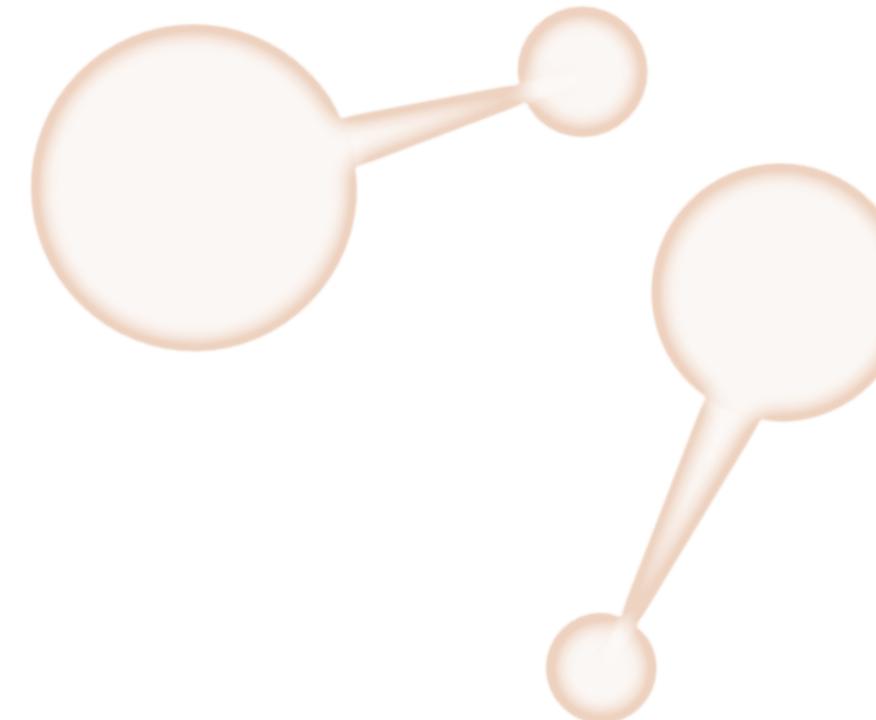


Internal Vibration

$$\Delta E \approx 300 \text{ cm}^{-1}$$

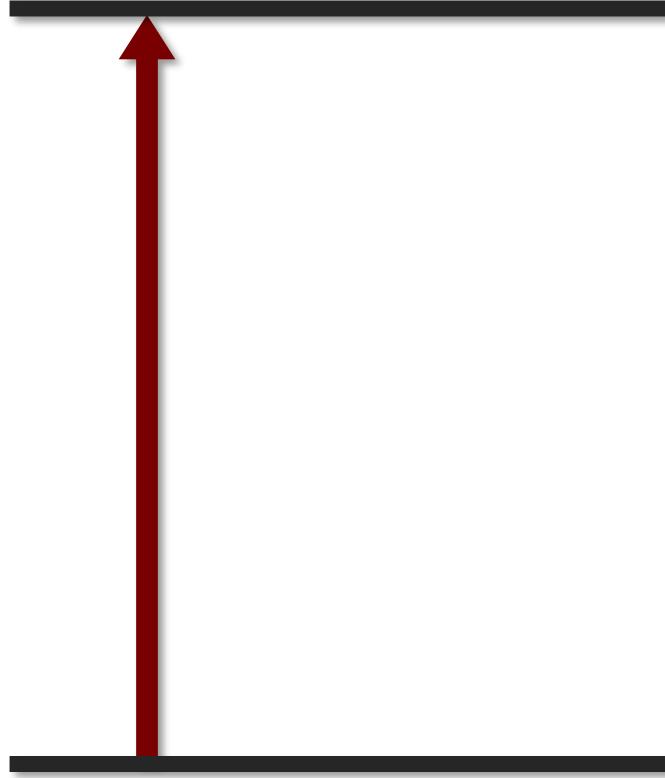


Pinned Rotation



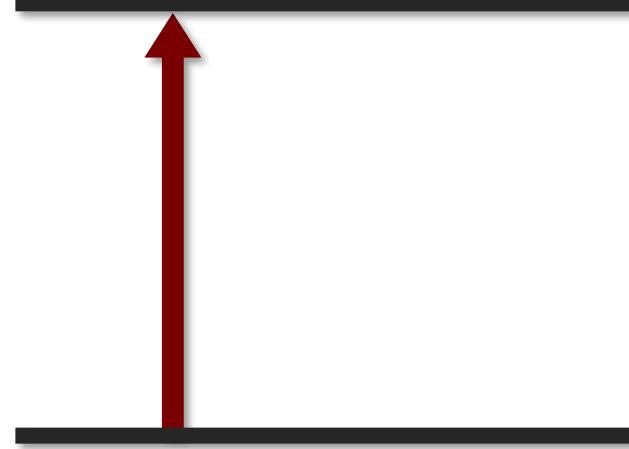
External Vibration

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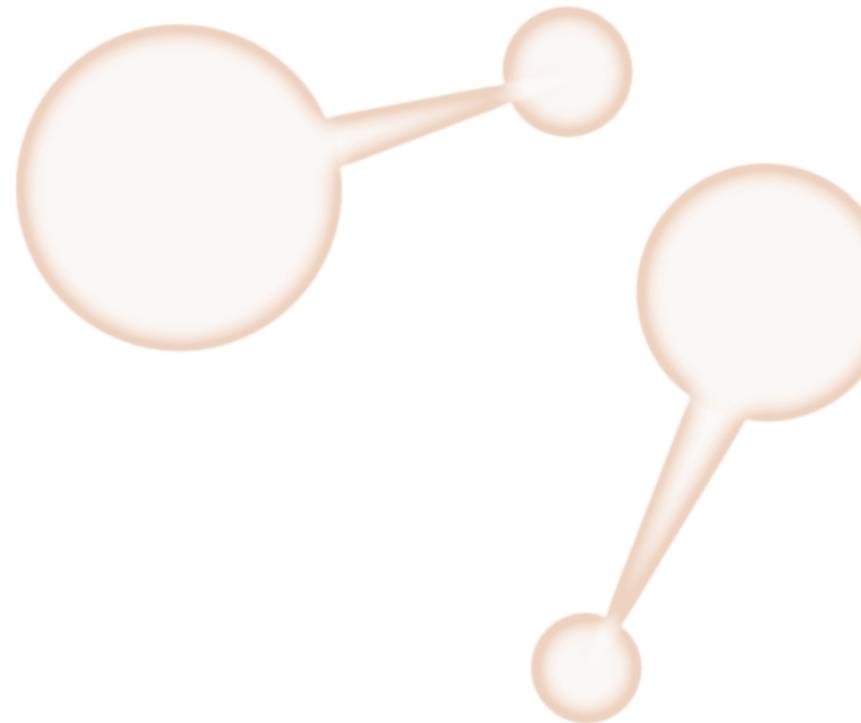


Internal Vibration

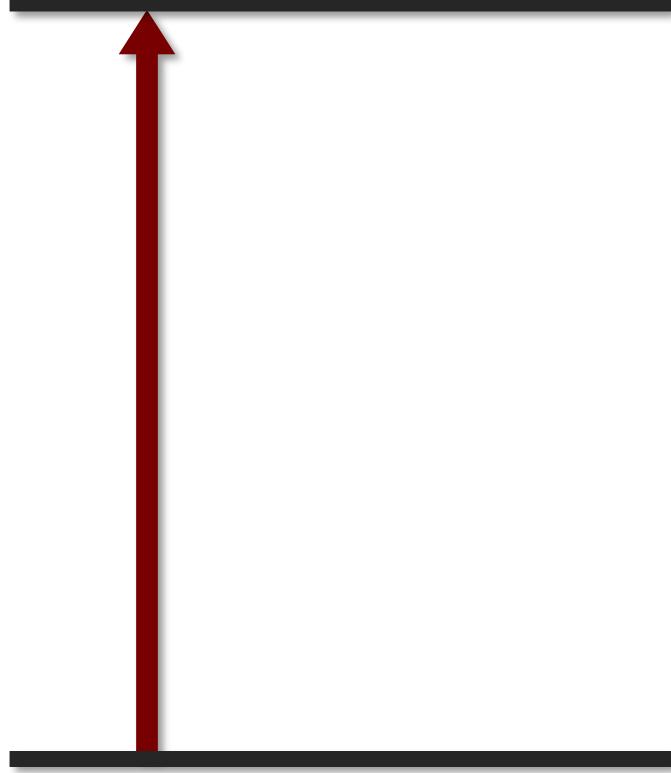
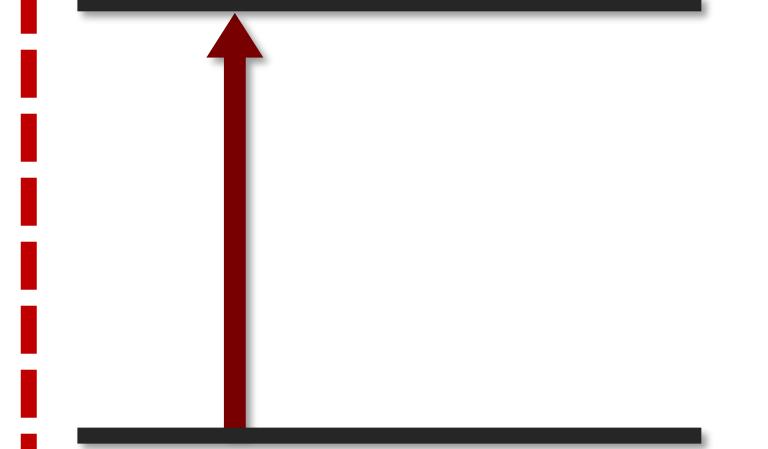
$$\Delta E \approx 300 \text{ cm}^{-1}$$



Pinned Rotation



External Vibration

$\Delta E \approx 4000 \text{ cm}^{-1}$ **Internal Vibration** $\Delta E \approx 300 \text{ cm}^{-1}$ **Pinned Rotation** $\Delta E \approx 5 \text{ cm}^{-1}$ **External Vibration**

$$H(R_{12}, R_{13}, R_{23}) = \sum_{i=1}^3 h_i + \sum_{i < j} V(r_i, r_j, \tilde{\theta}_i, \tilde{\theta}_j, \tilde{\phi}; R_{ij})^*$$

$$\langle I | \hat{H} | J \rangle \Rightarrow \{E_0, E_1, E_2, \dots\}$$

$$|I\rangle = \prod_{i=1}^N |\Phi_i\rangle \quad |\Phi\rangle = |lm\rangle \otimes |lv\rangle = |lmv\rangle$$

$$\hat{h}|lv\rangle = \varepsilon_v^l|lv\rangle \quad \hat{L}^2|lm\rangle = l(l+1)|lm\rangle \quad \hat{L}_z|lm\rangle = m^2|lm\rangle$$

*R. J. Hinde, J. Chem. Phys. **128**, 154308 (2008)

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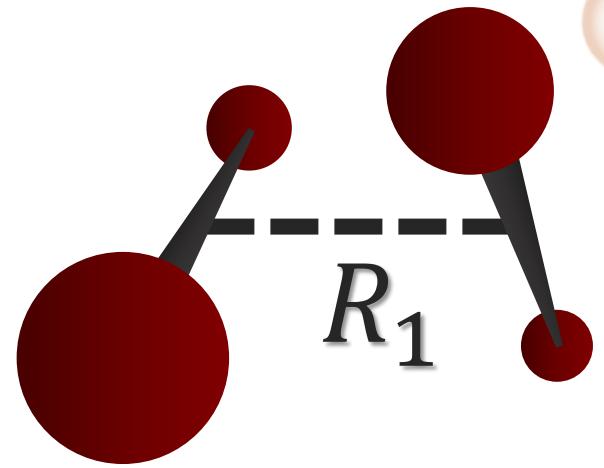
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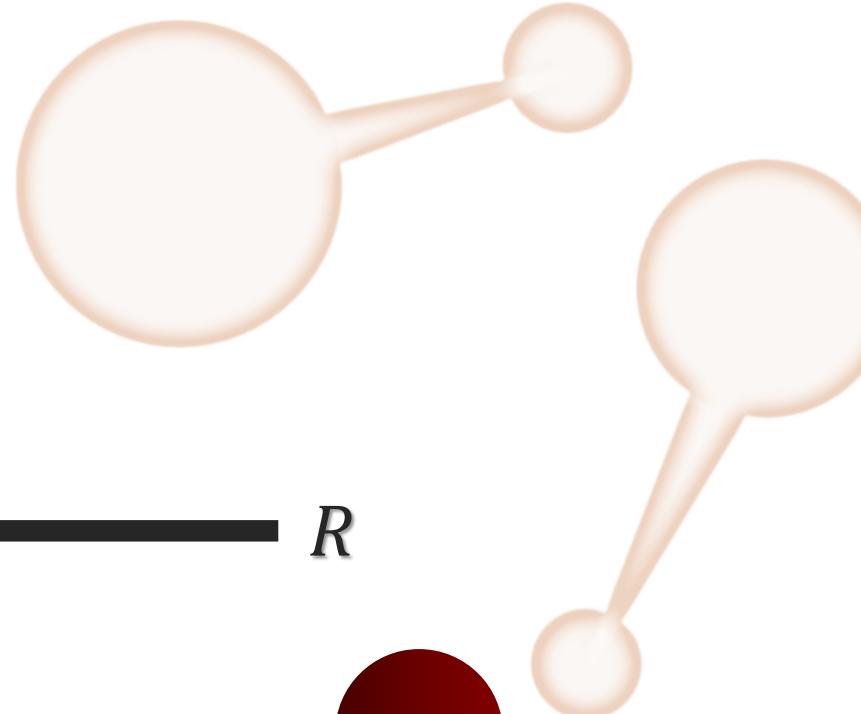
*R. J. Hinde, J. Chem. Phys. **128**, 154308 (2008)

$V(R)$

R



R_1



Conclusions

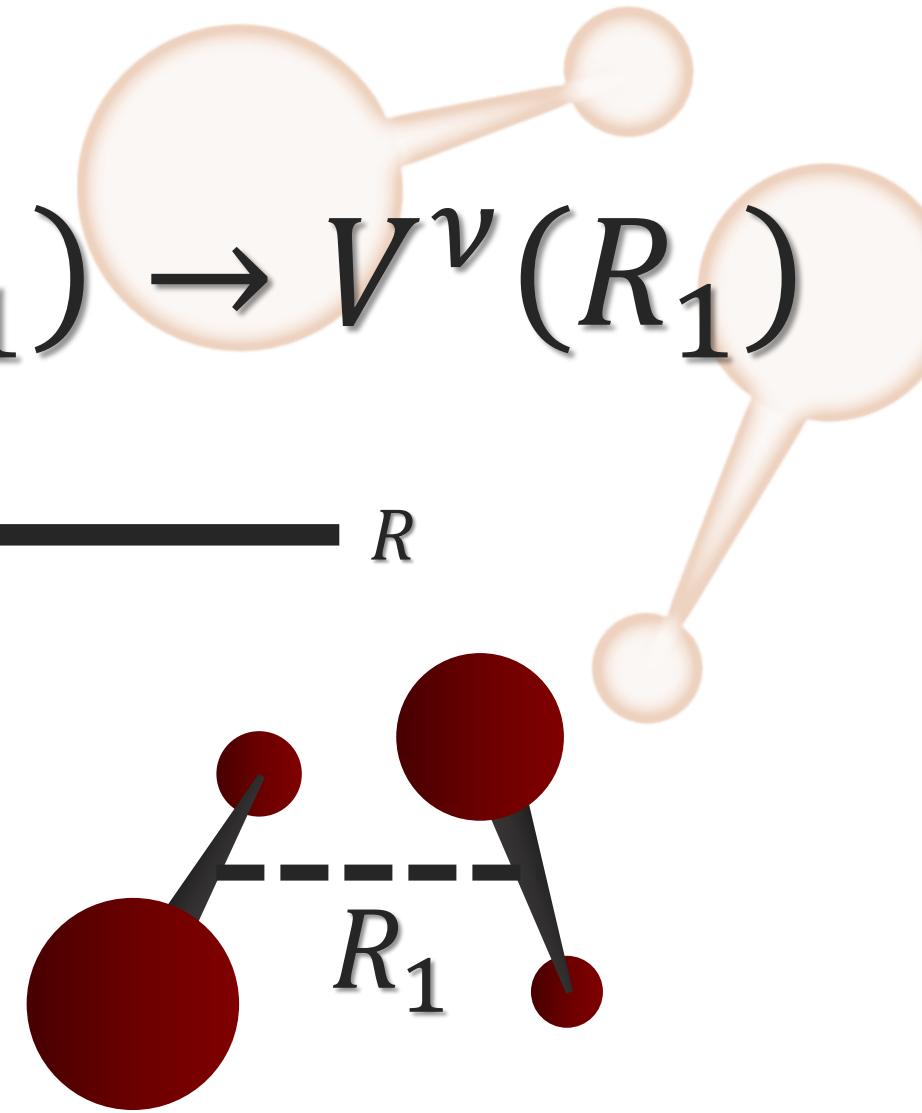
Confined Water

Dipole Chains

Hydrogen Clusters

Overview

$$\langle I | \hat{H}(R_1) | J \rangle \rightarrow E_0^\nu(R_1) \rightarrow V^\nu(R_1)$$



$$V(R)$$

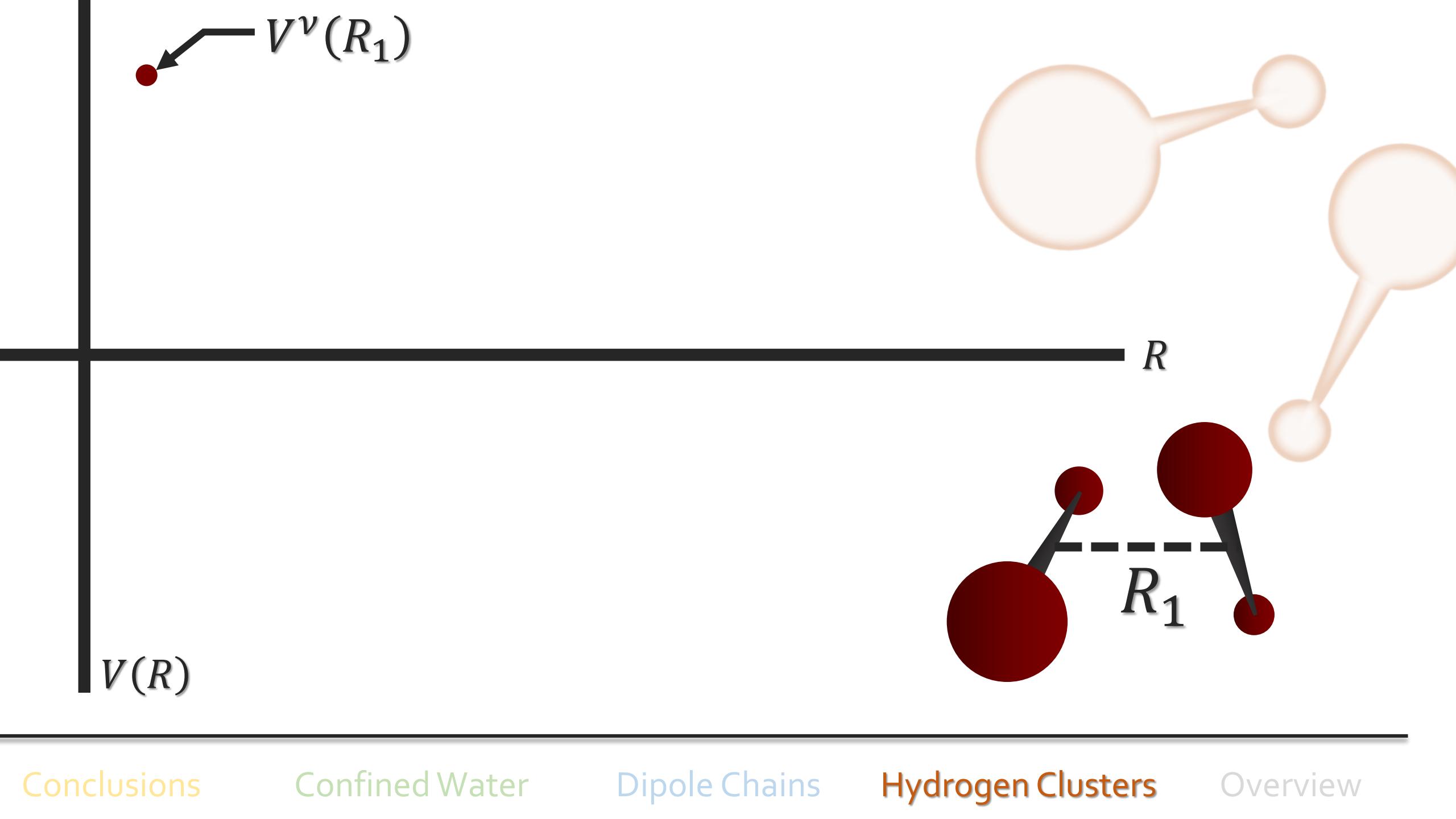
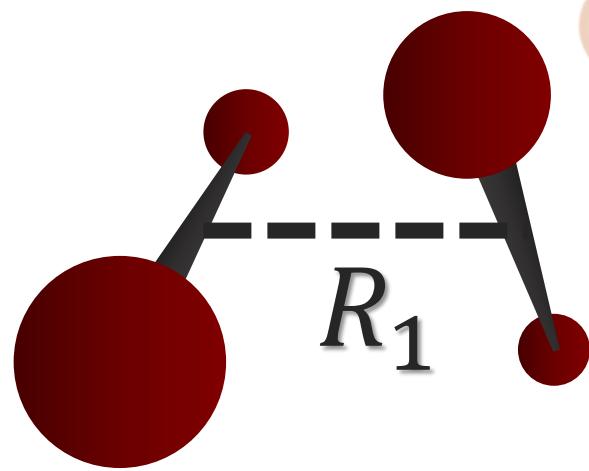
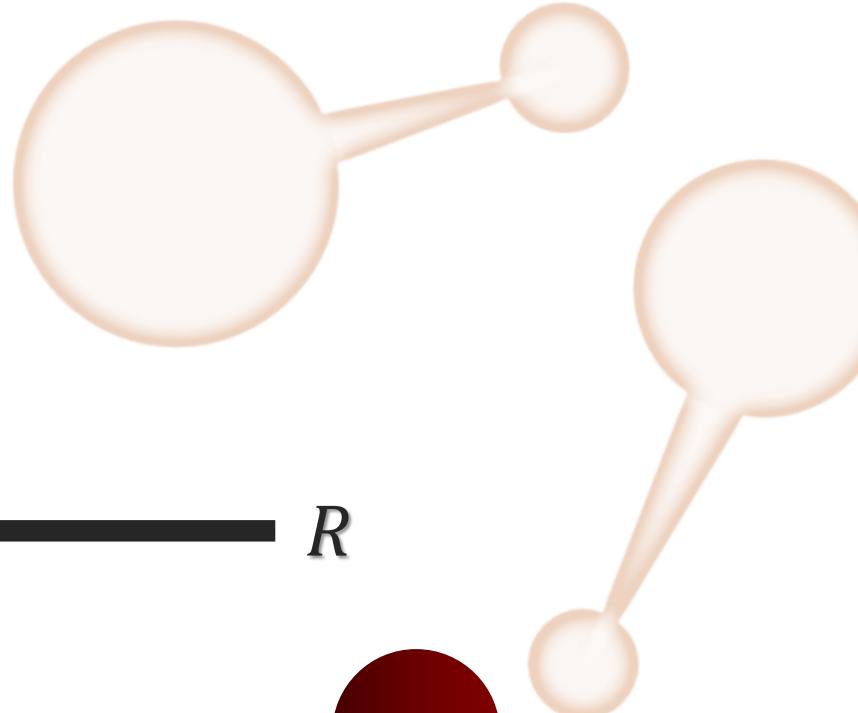
Conclusions

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 $V^v(R_1)$ 

$V(R)$

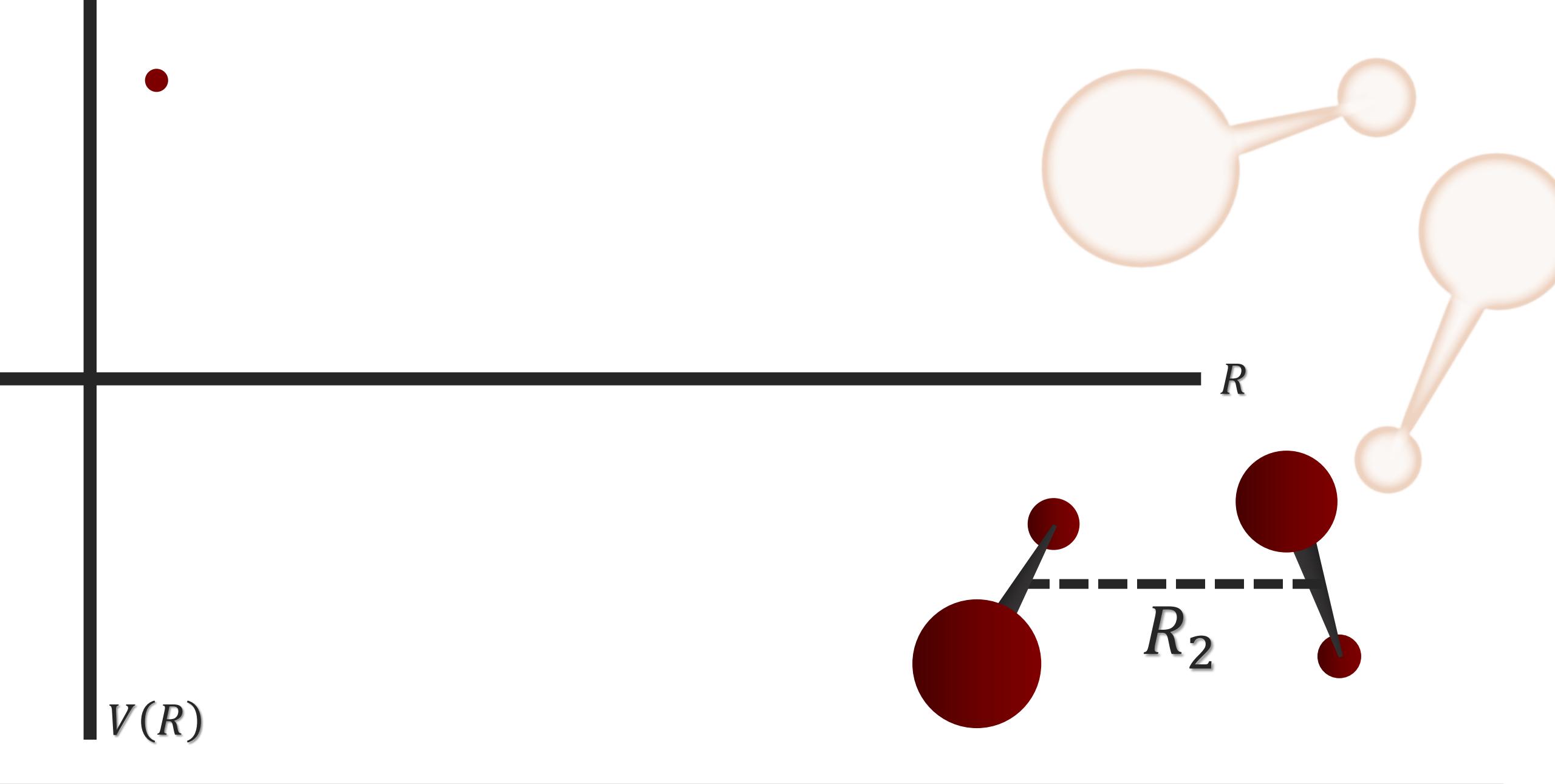
Conclusions

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Conclusions

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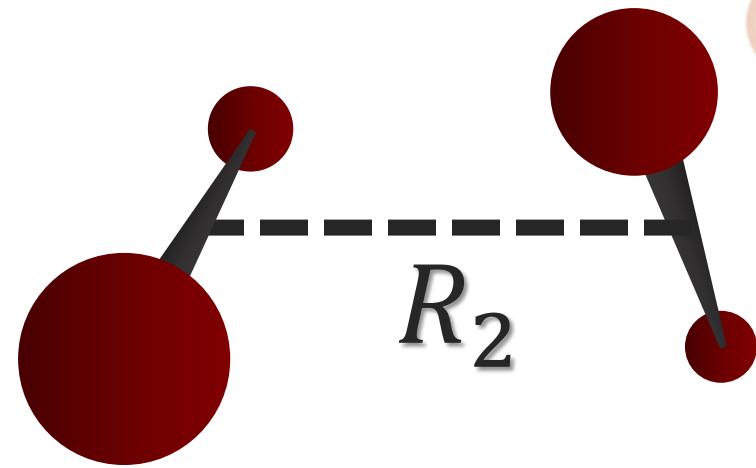
Overview

•

$$\langle I | \hat{H}(R_2) | J \rangle \rightarrow E_0^\nu(R_2) \rightarrow V^\nu(R_2)$$

R

$V(R)$



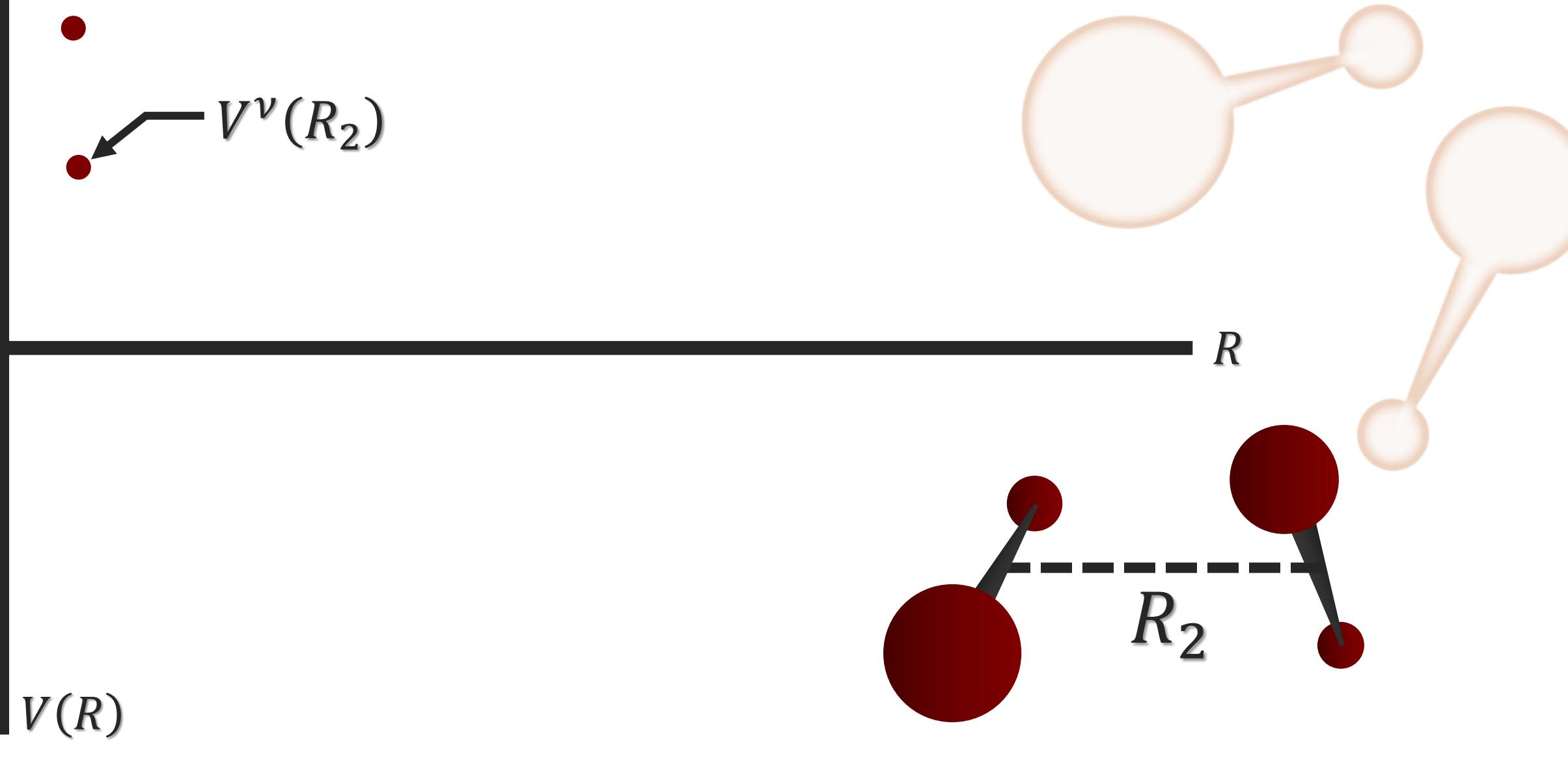
Conclusions

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Overview



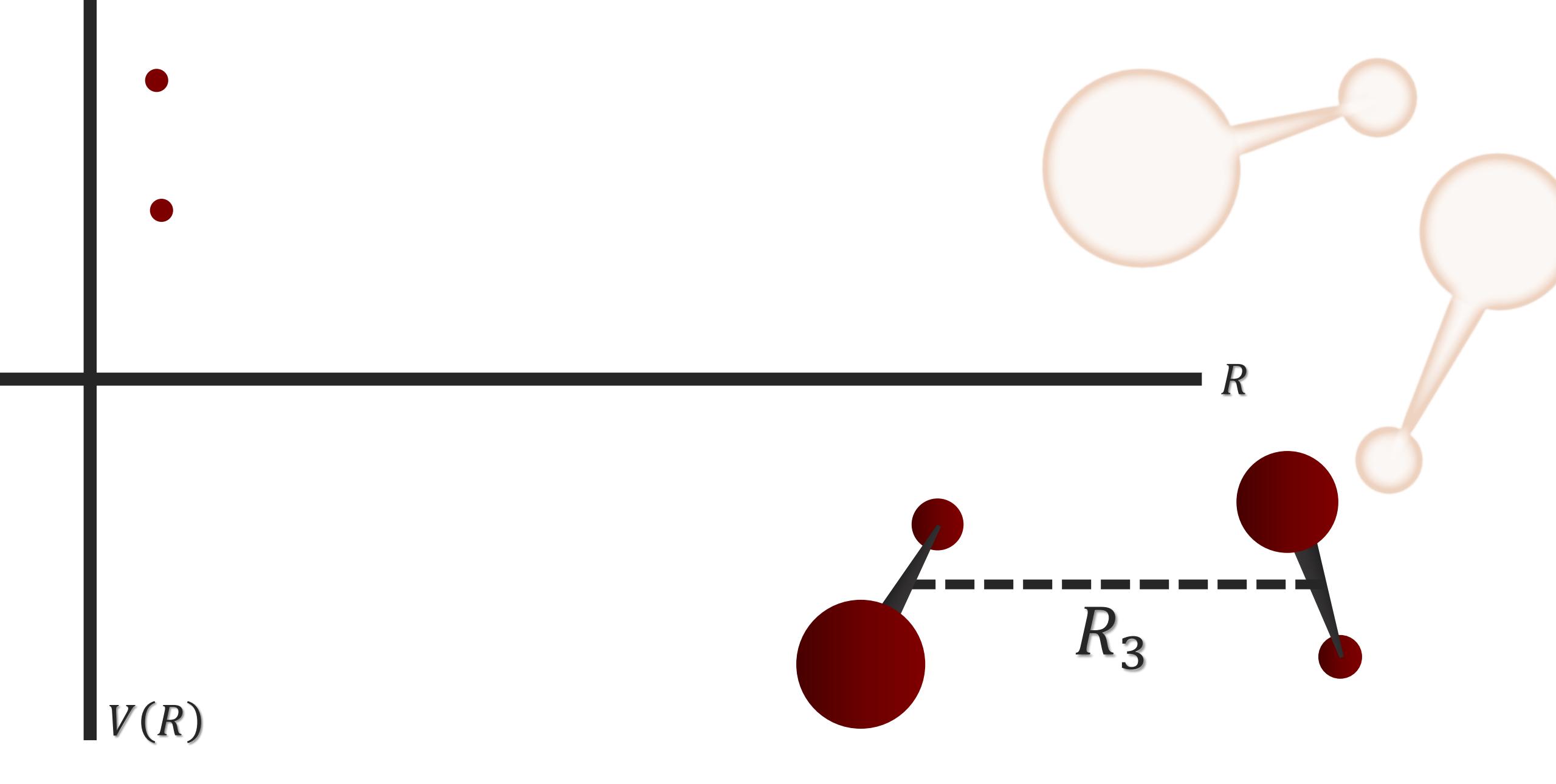
Conclusions

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Conclusions

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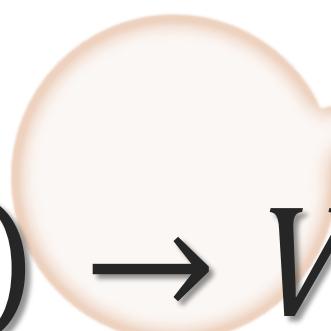
Overview

•

$$\langle I | \hat{H}(R_3) | J \rangle$$

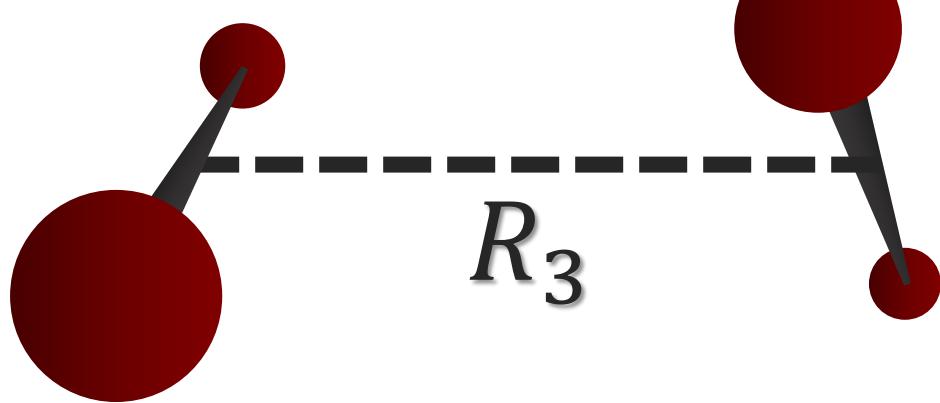
\rightarrow

$$E_0^\nu(R_3)$$

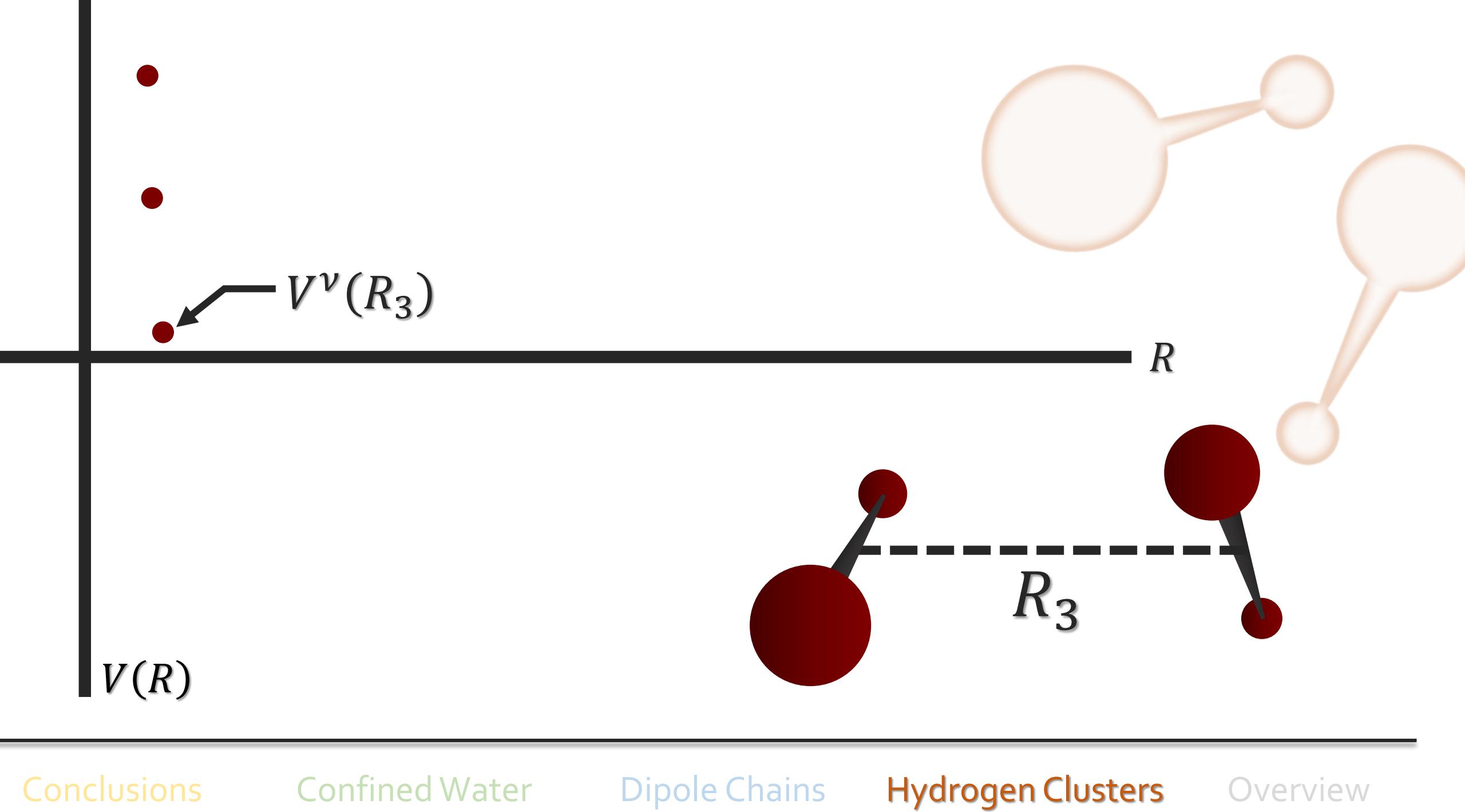


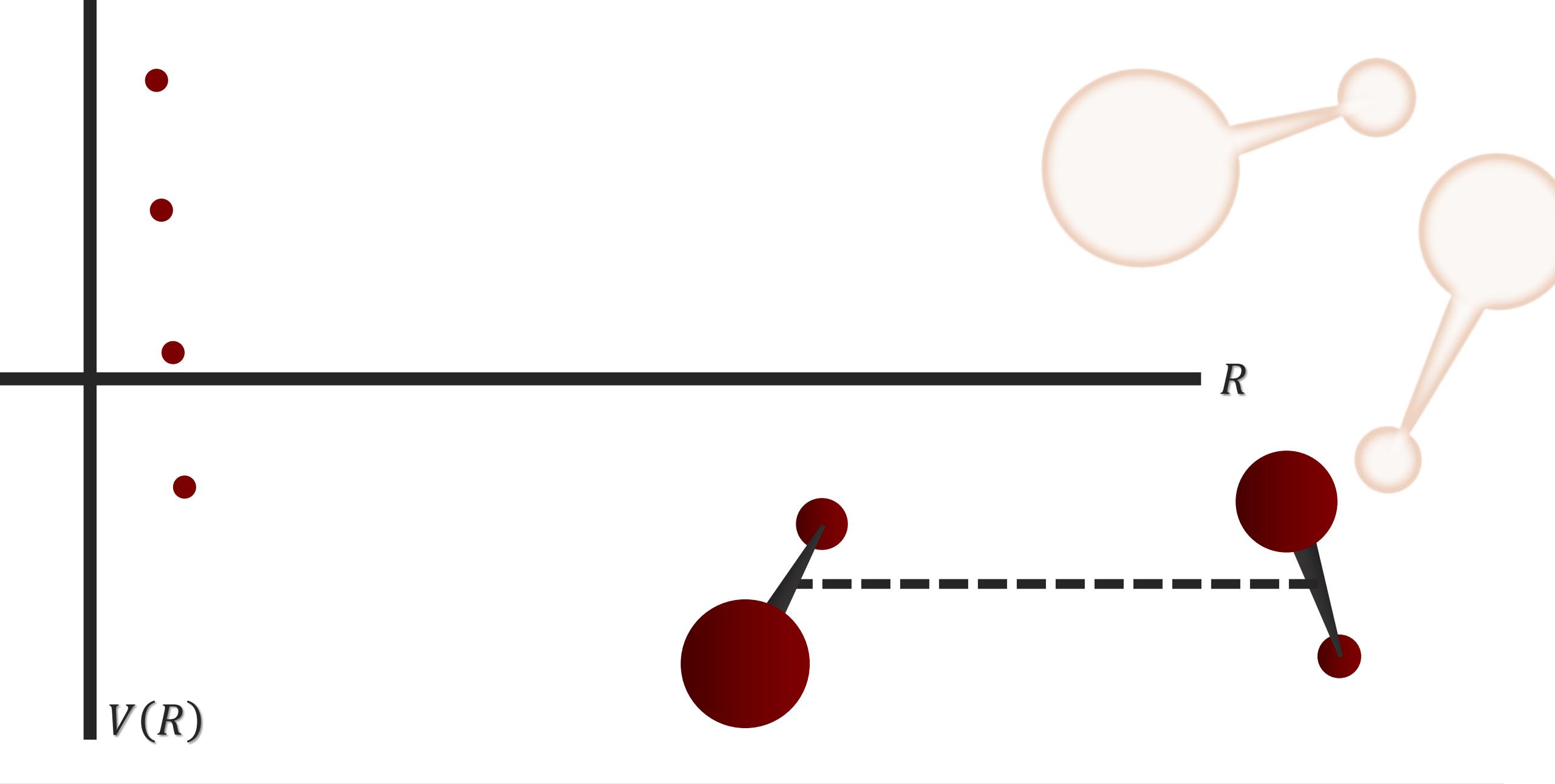
$$\rightarrow V^\nu(R_3)$$

R



$$V(R)$$





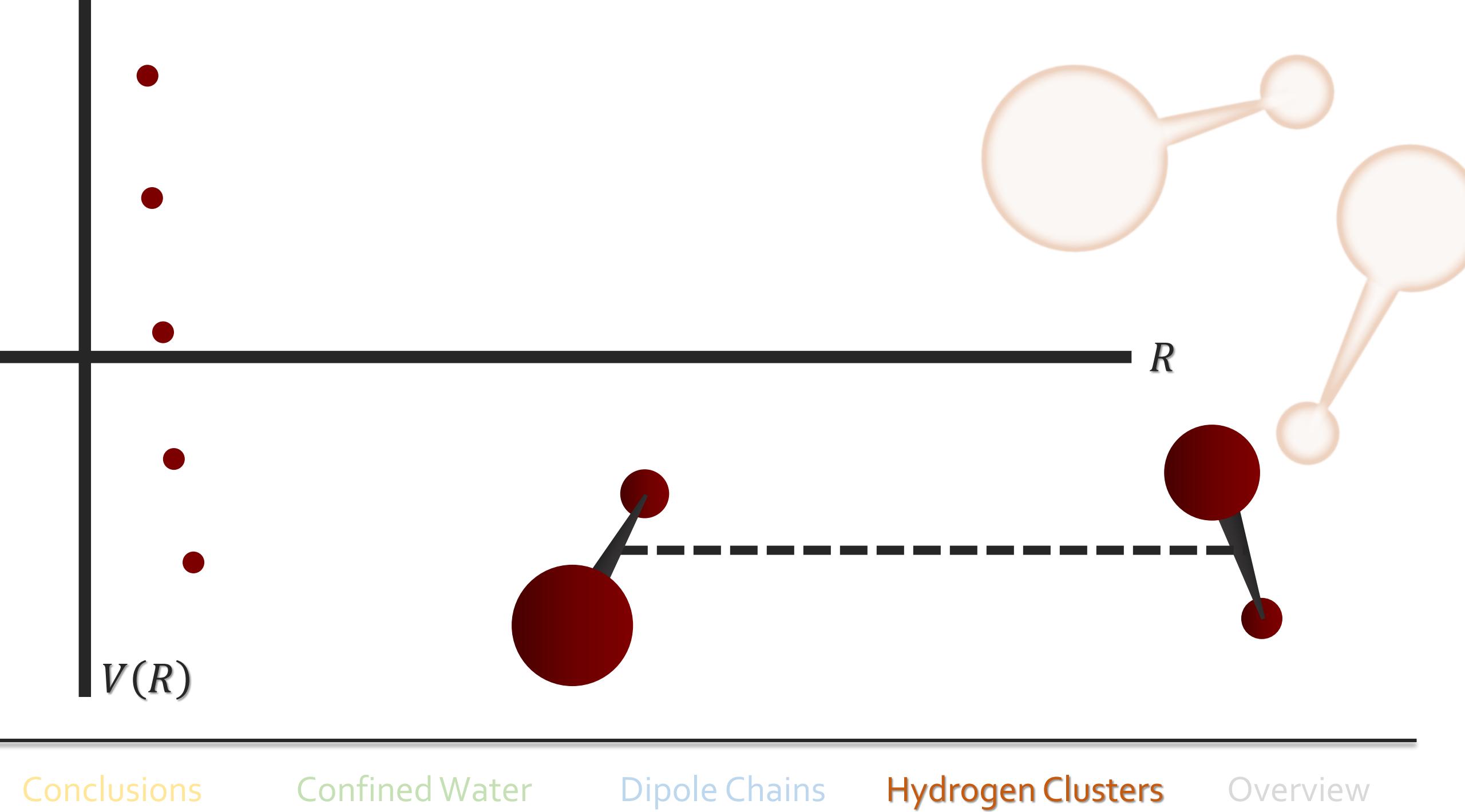
Conclusions

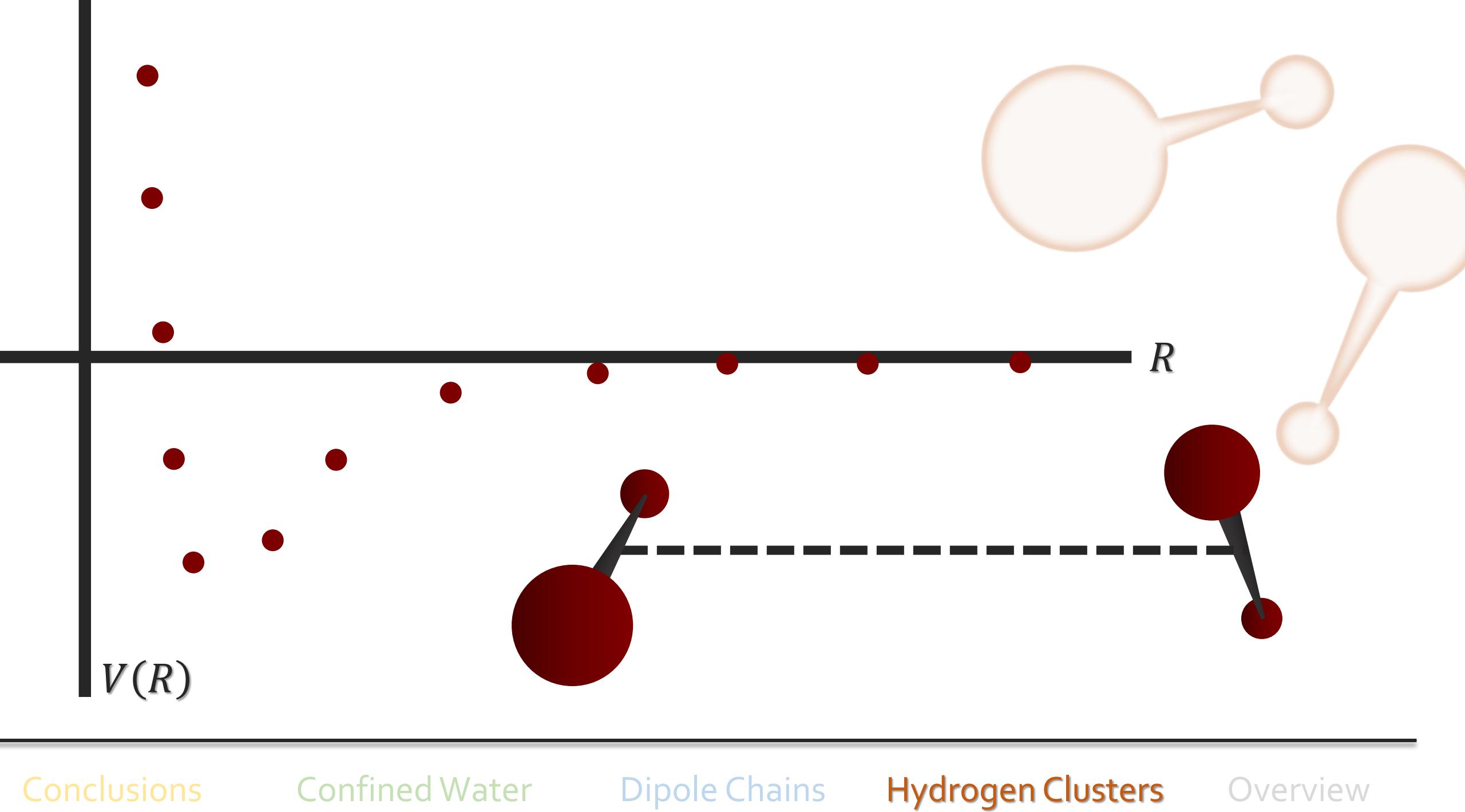
Confined Water

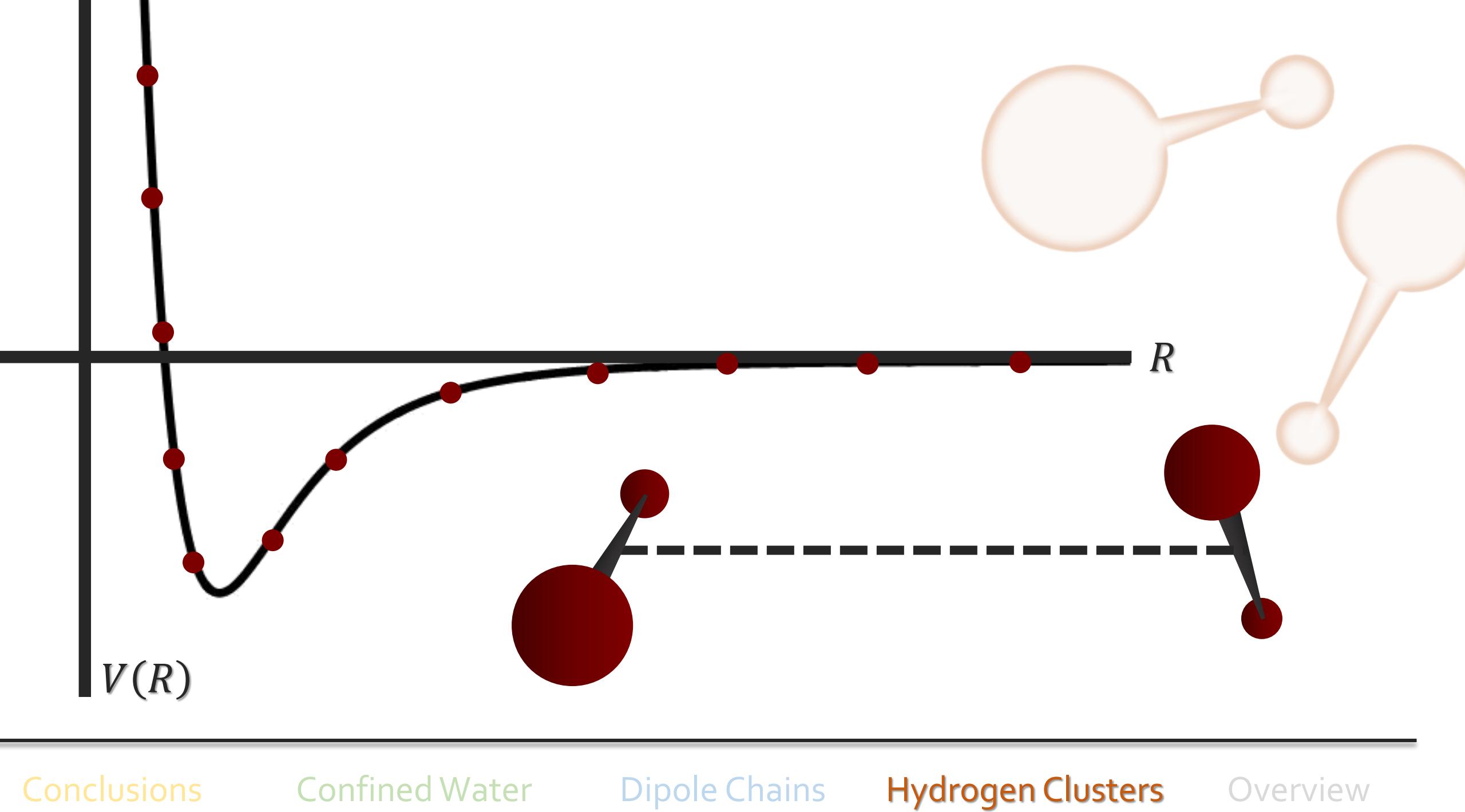
Dipole Chains

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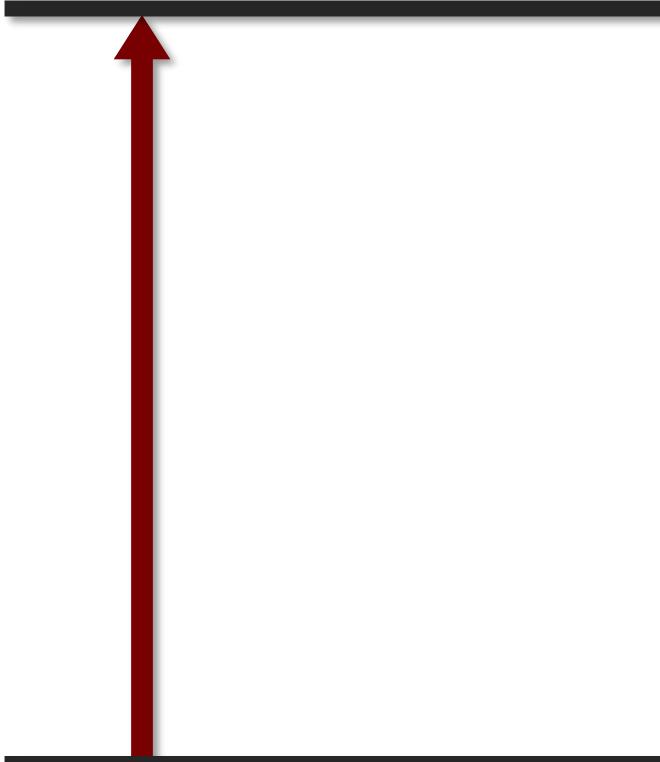
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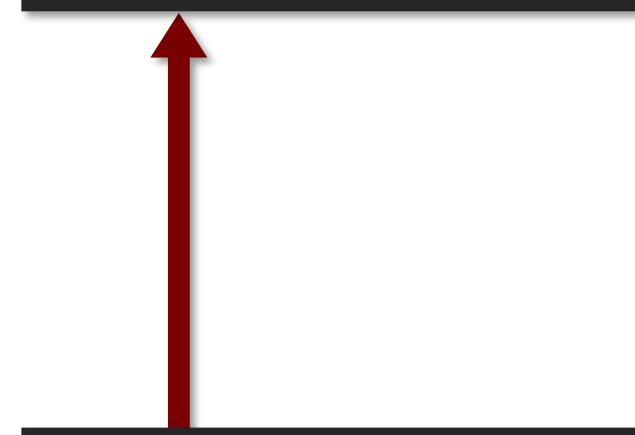
Overview

$$\Delta E \approx 4000 \text{ cm}^{-1}$$

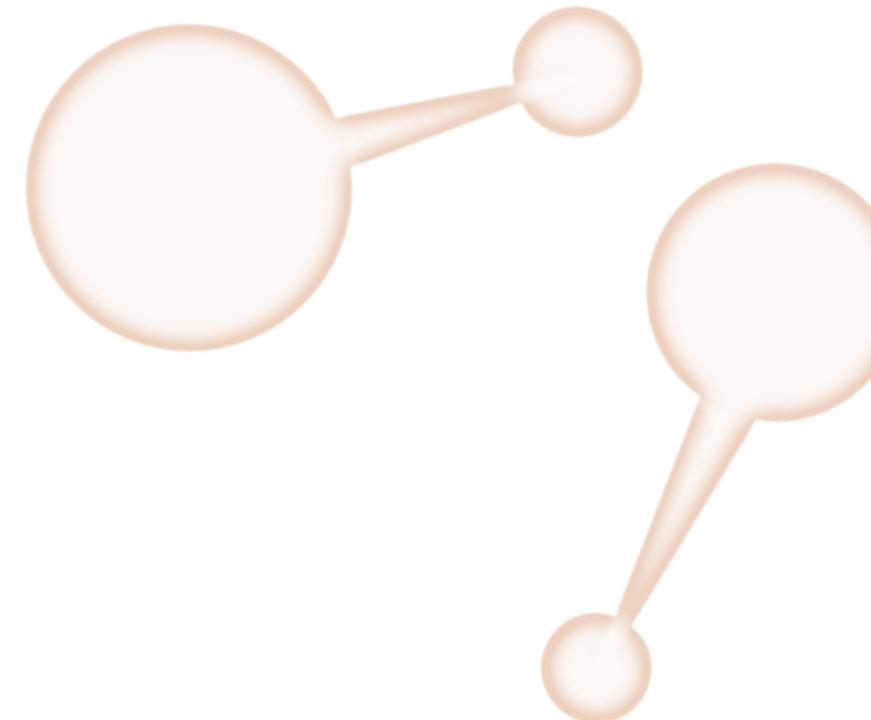


Internal Vibration

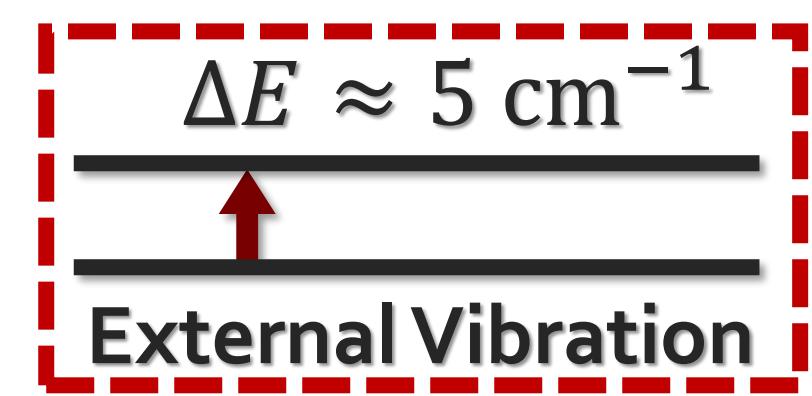
$$\Delta E \approx 300 \text{ cm}^{-1}$$



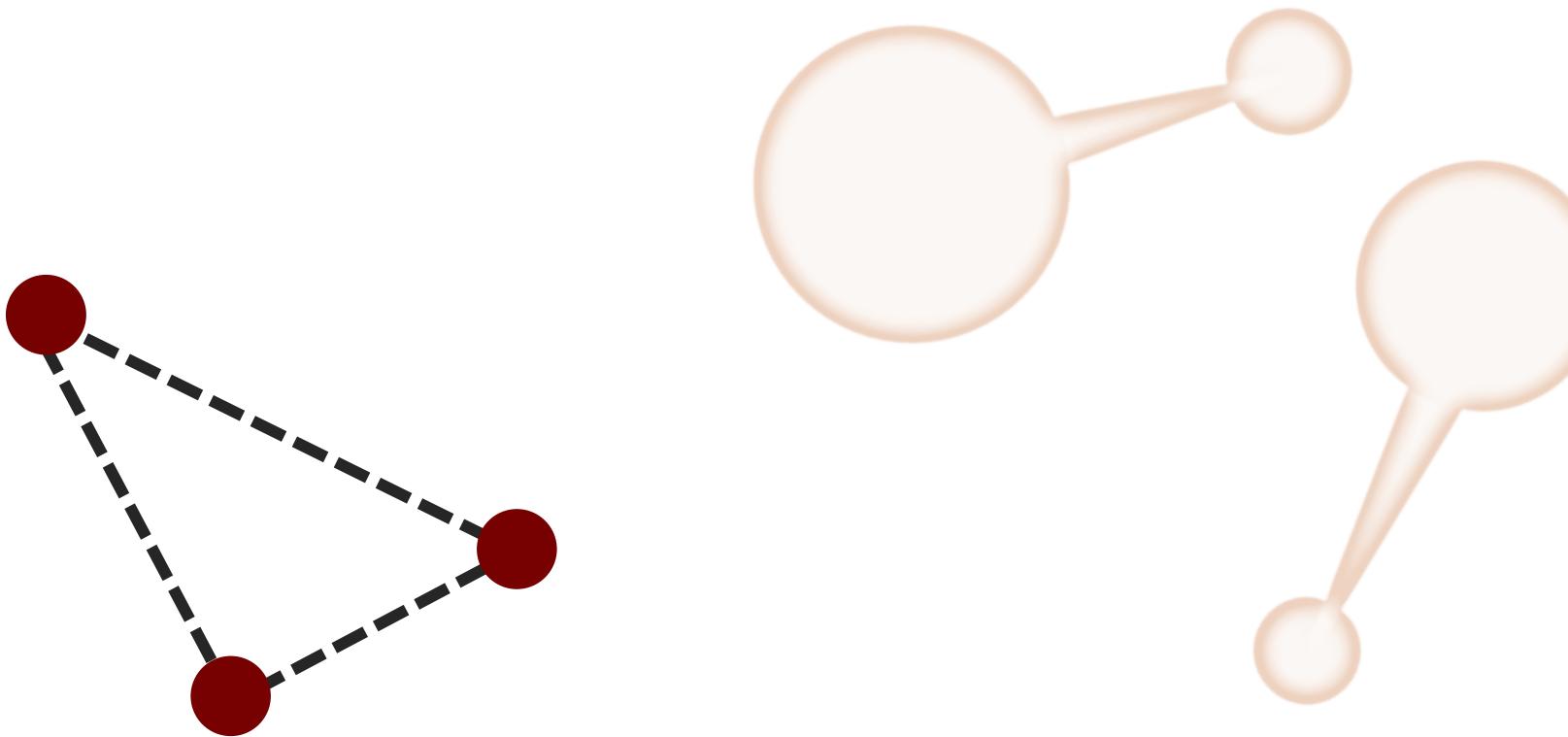
Pinned Rotation

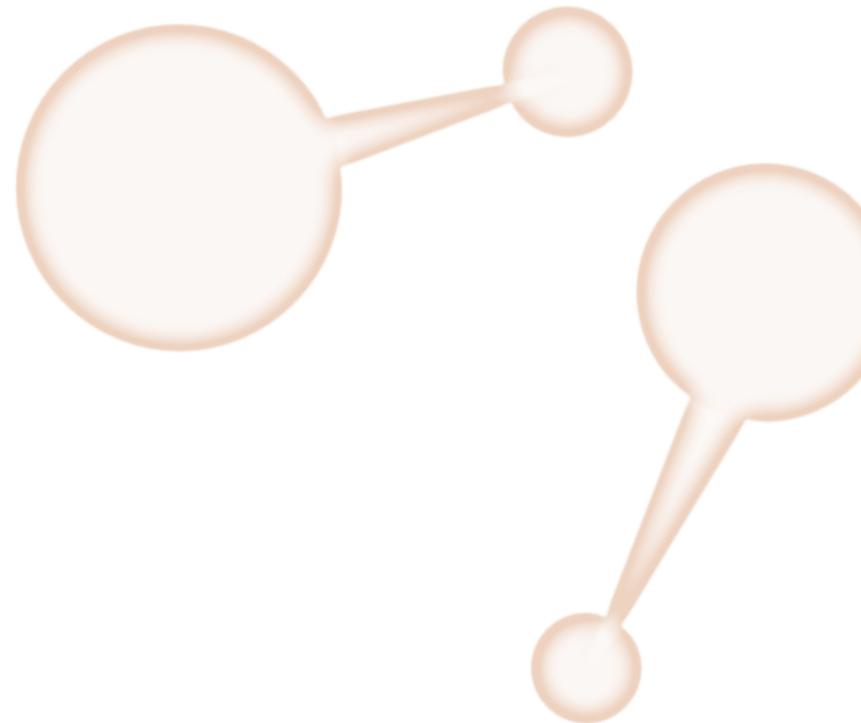
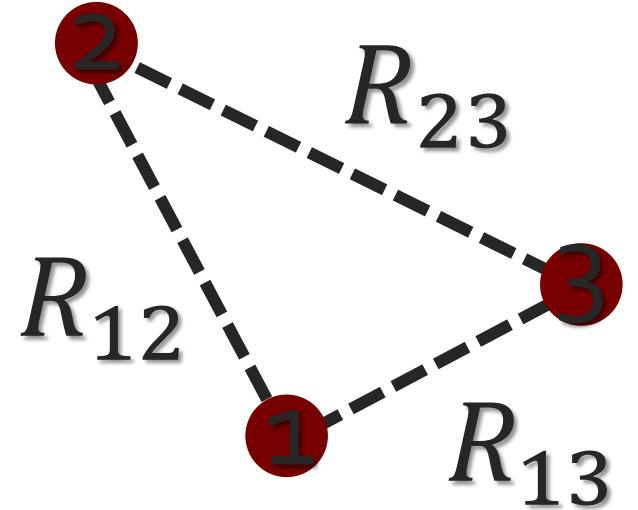


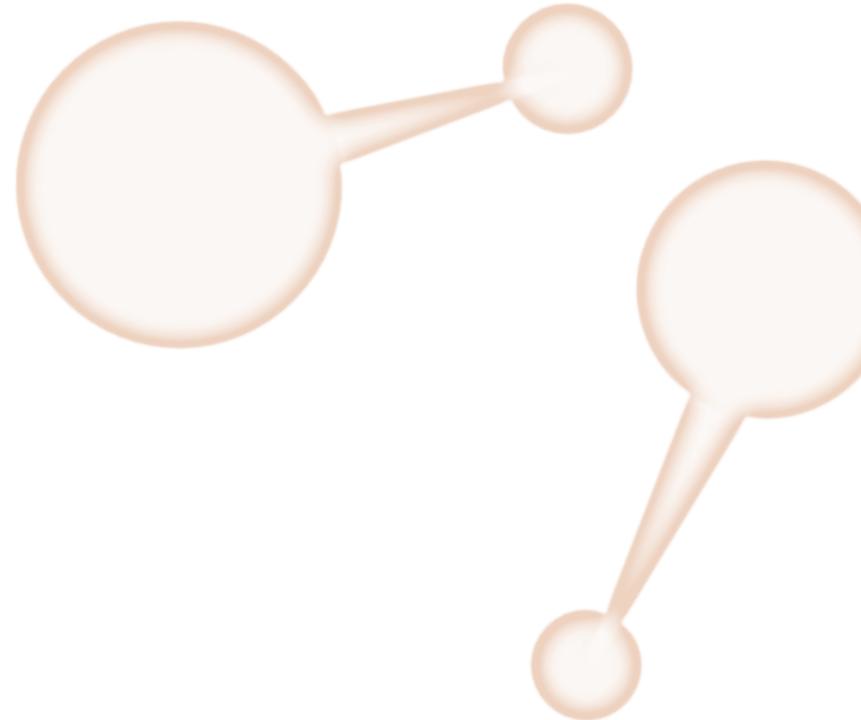
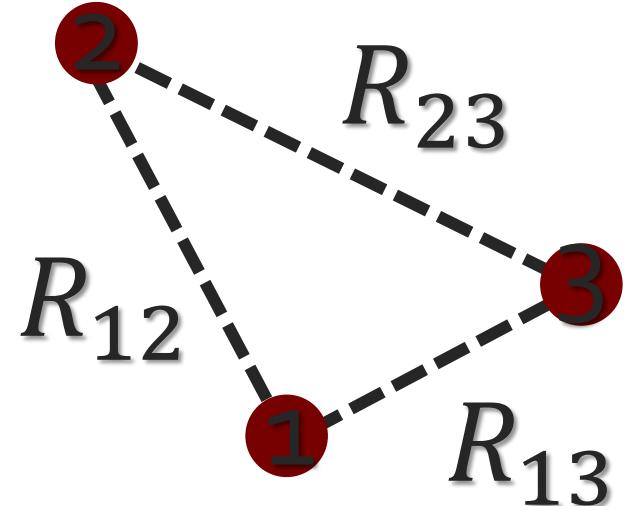
$$\Delta E \approx 5 \text{ cm}^{-1}$$



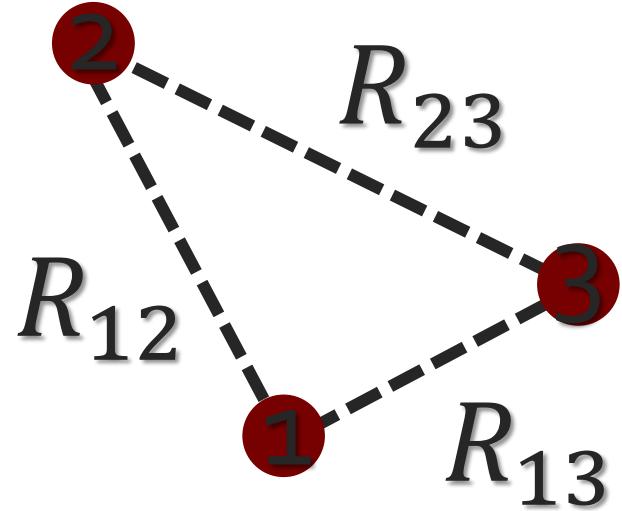
External Vibration





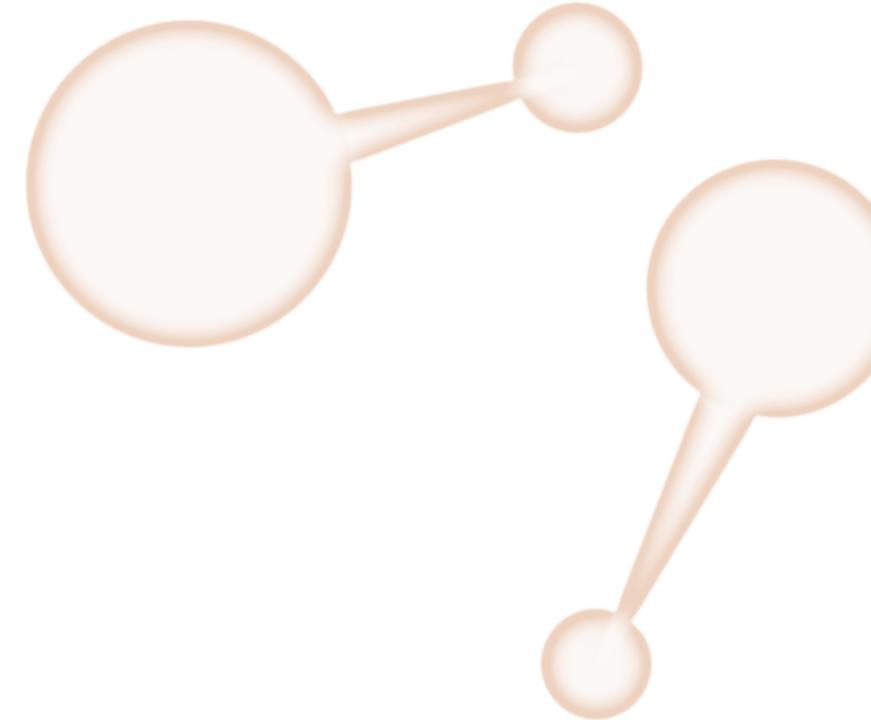


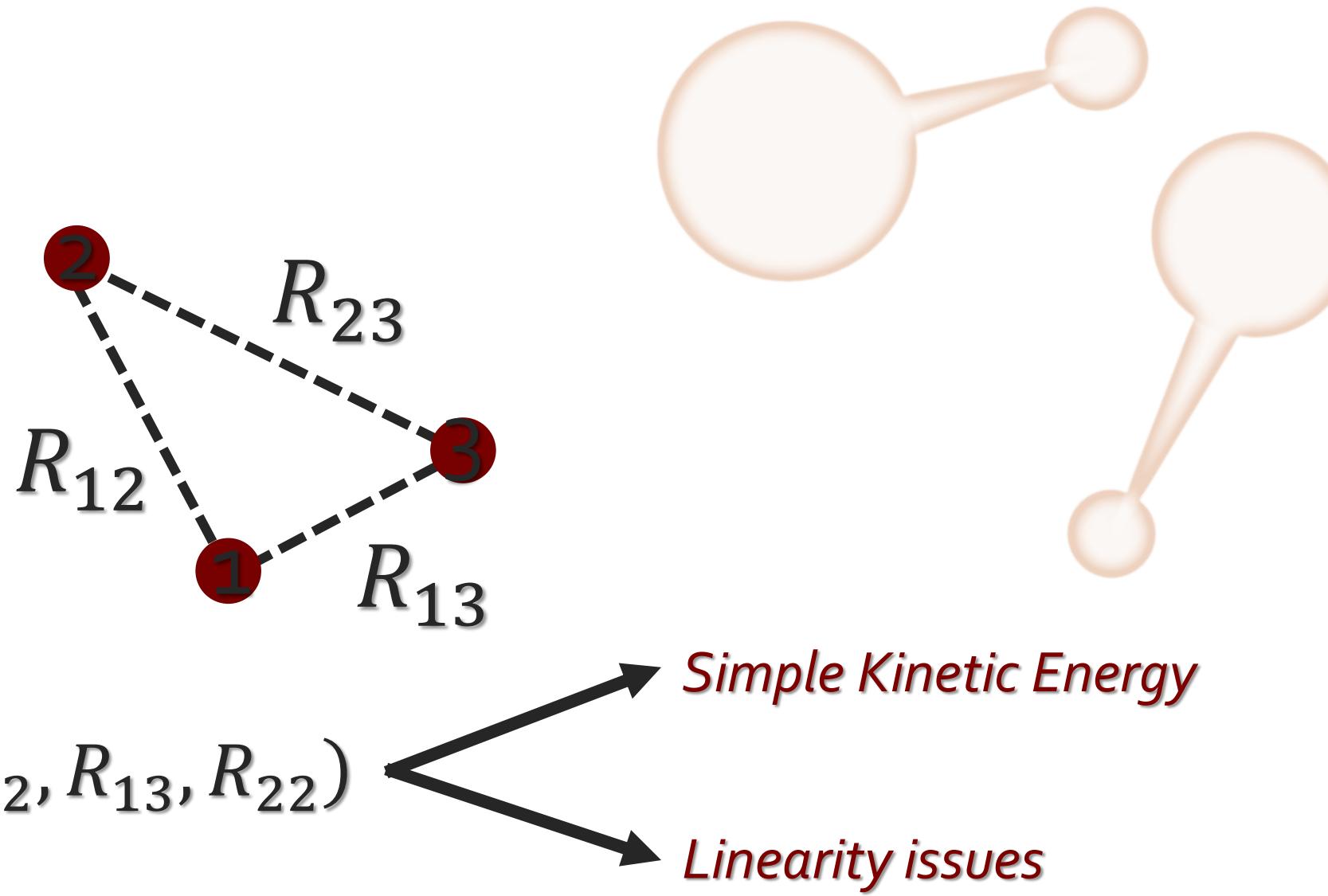
$$V = V(R_{12}, R_{13}, R_{23})$$

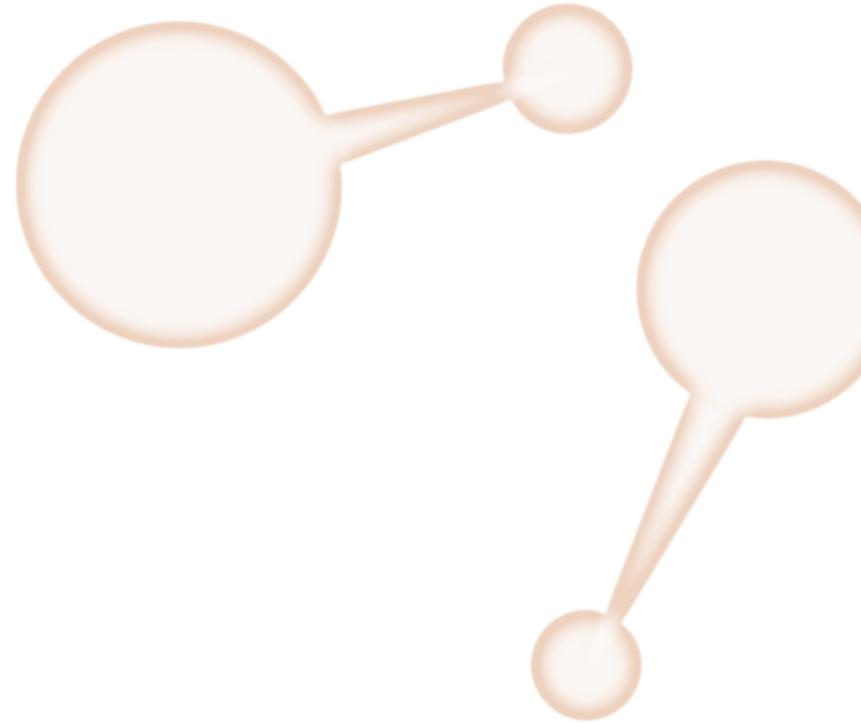
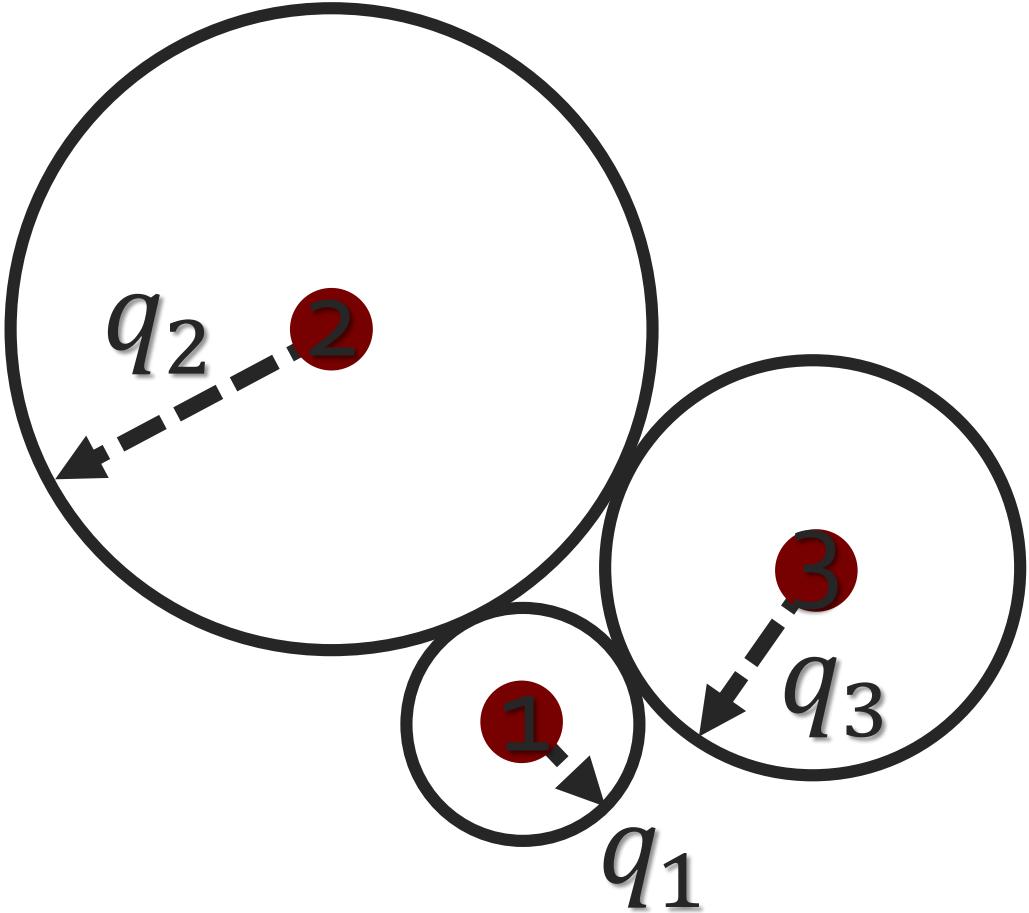


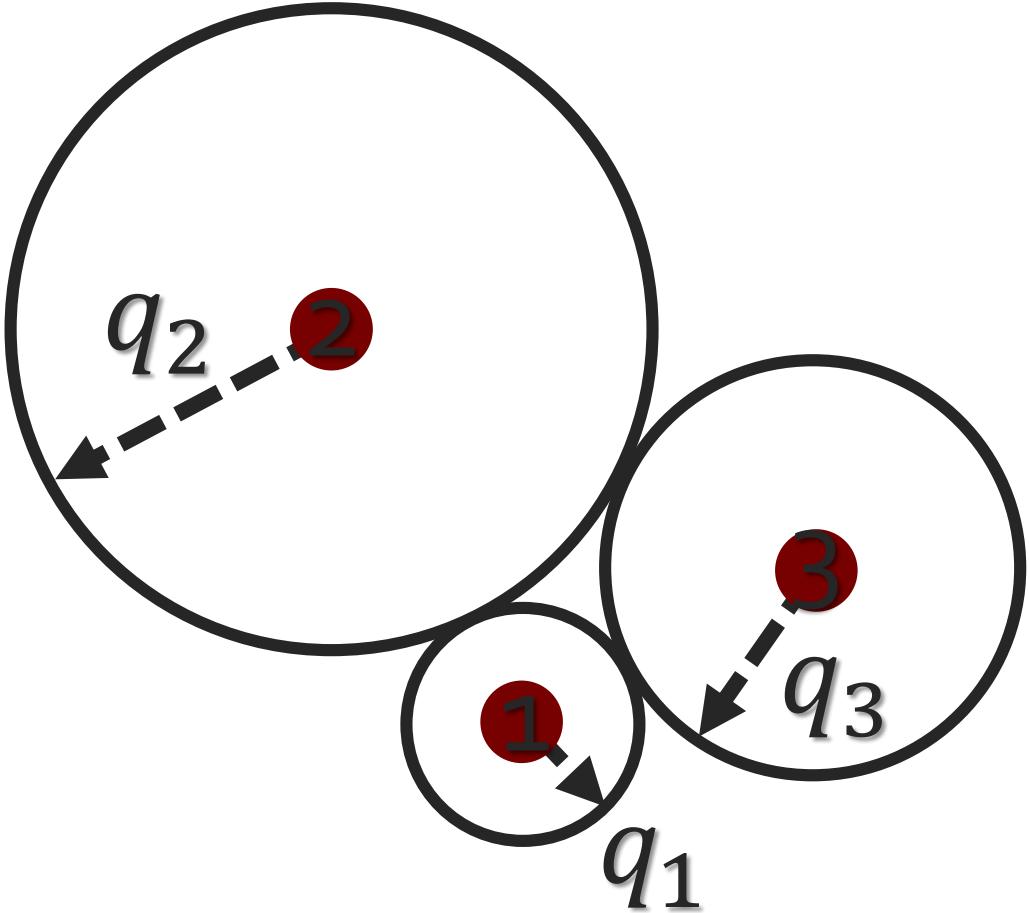
$$V = V(R_{12}, R_{13}, R_{23})$$

Simple Kinetic Energy

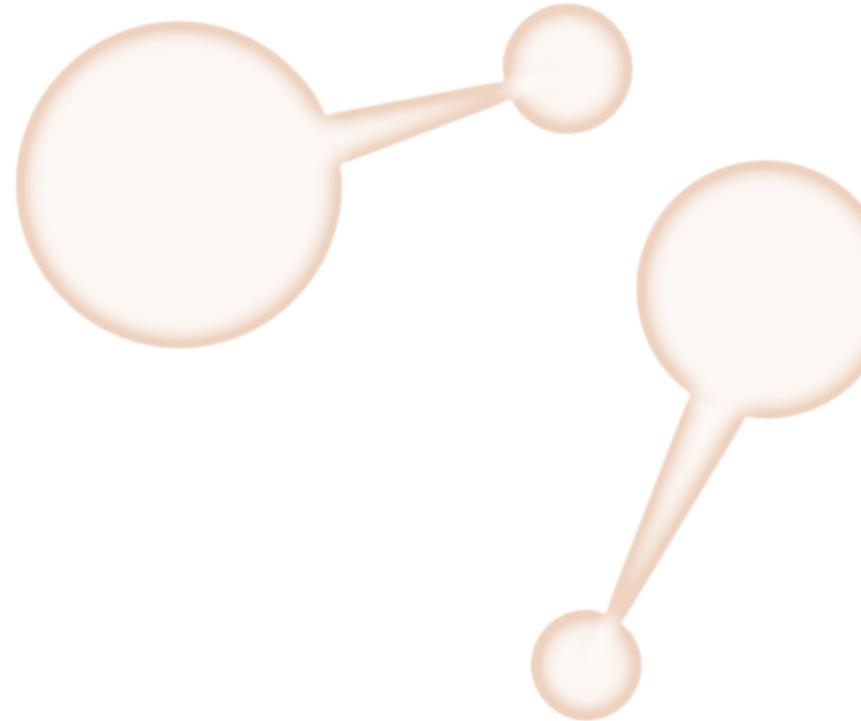


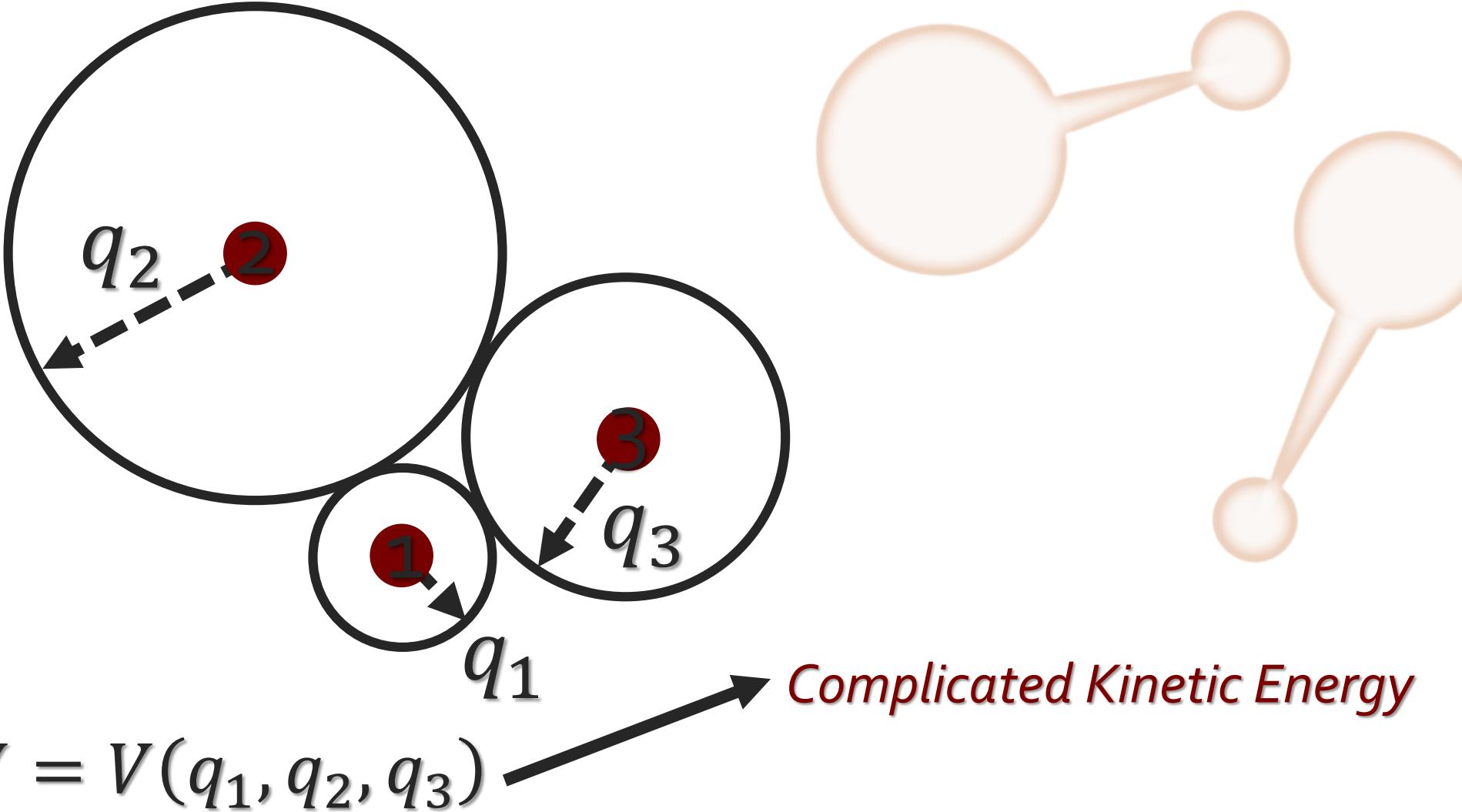


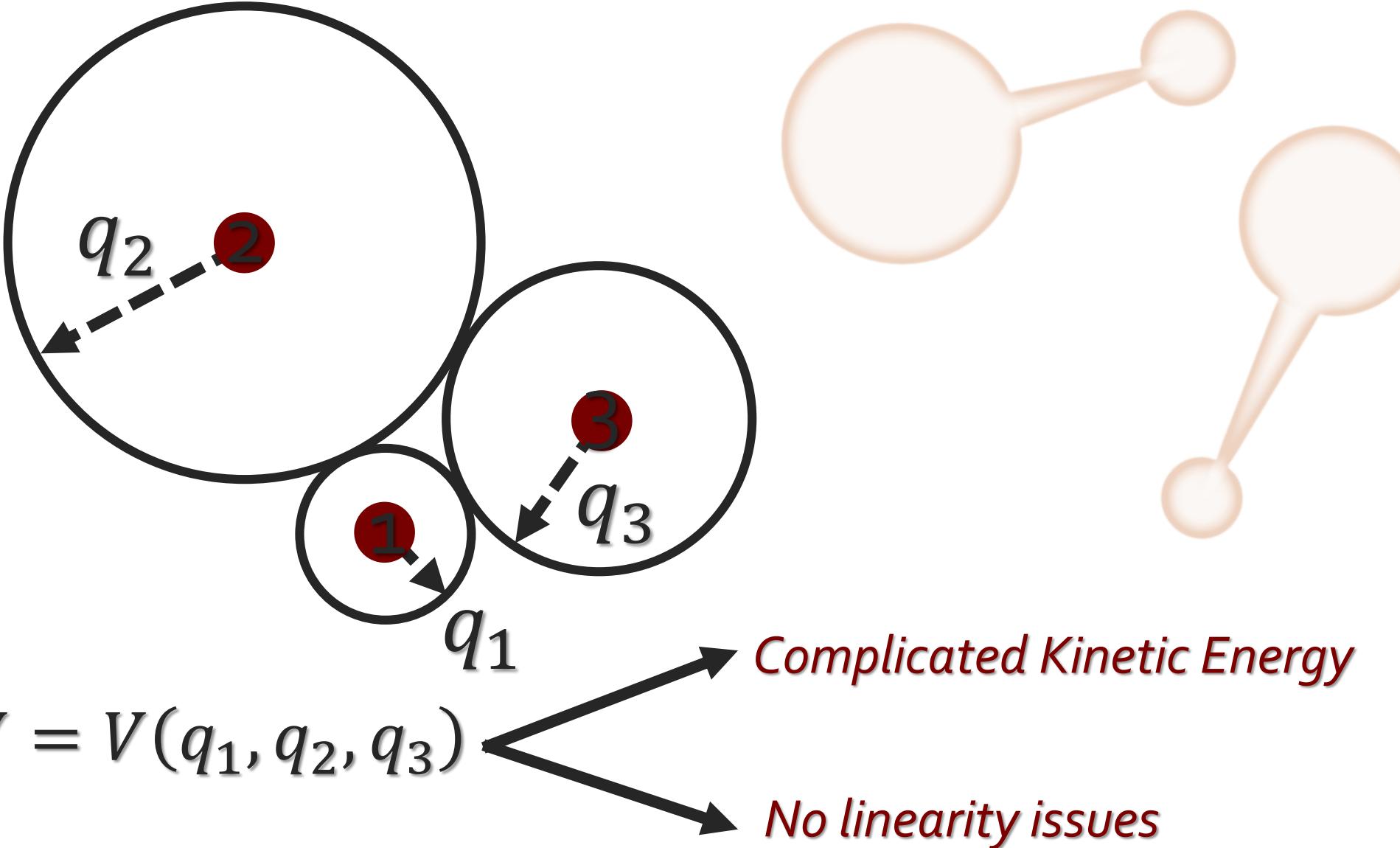


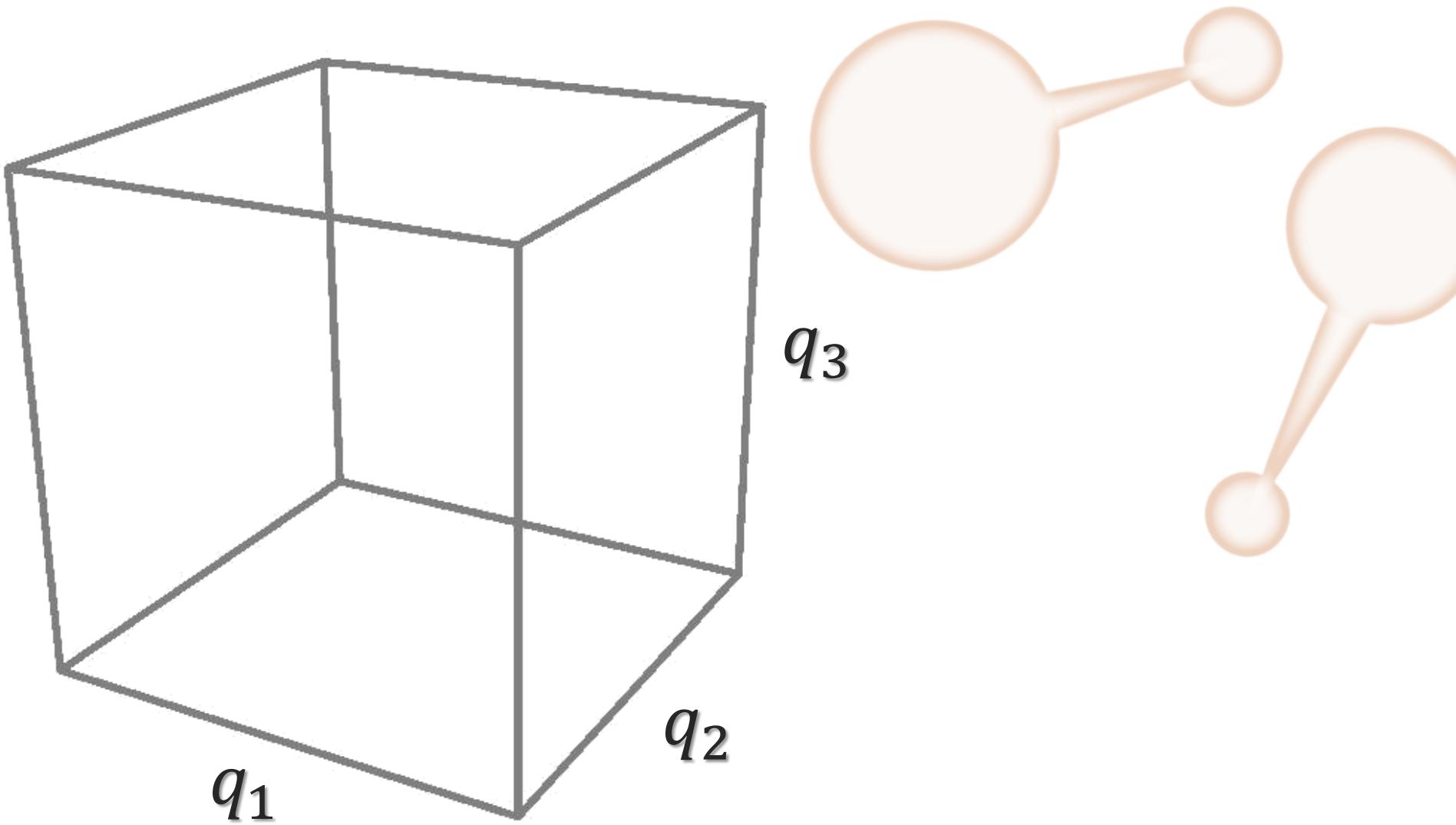


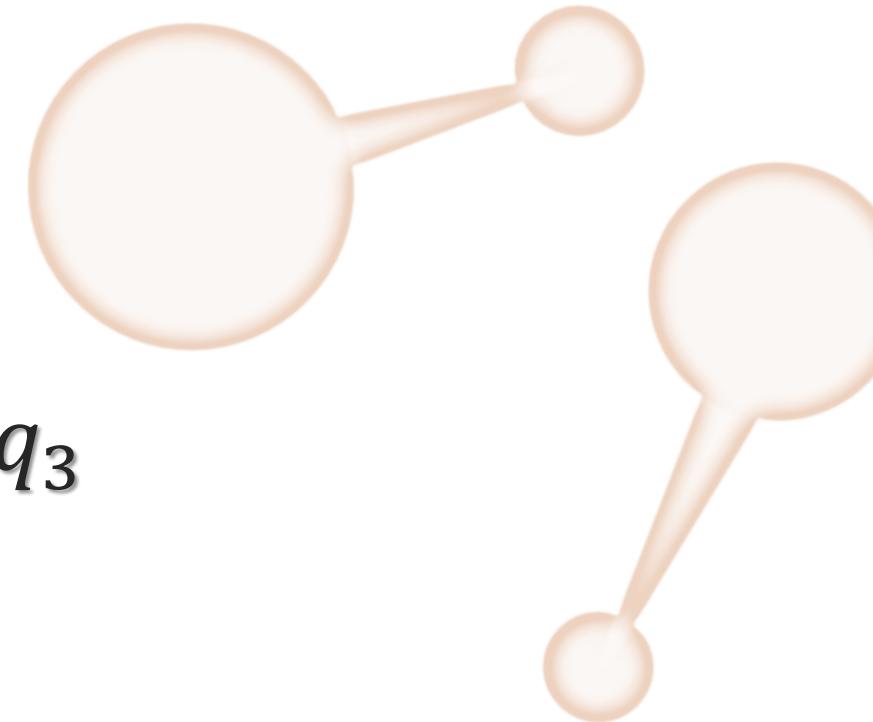
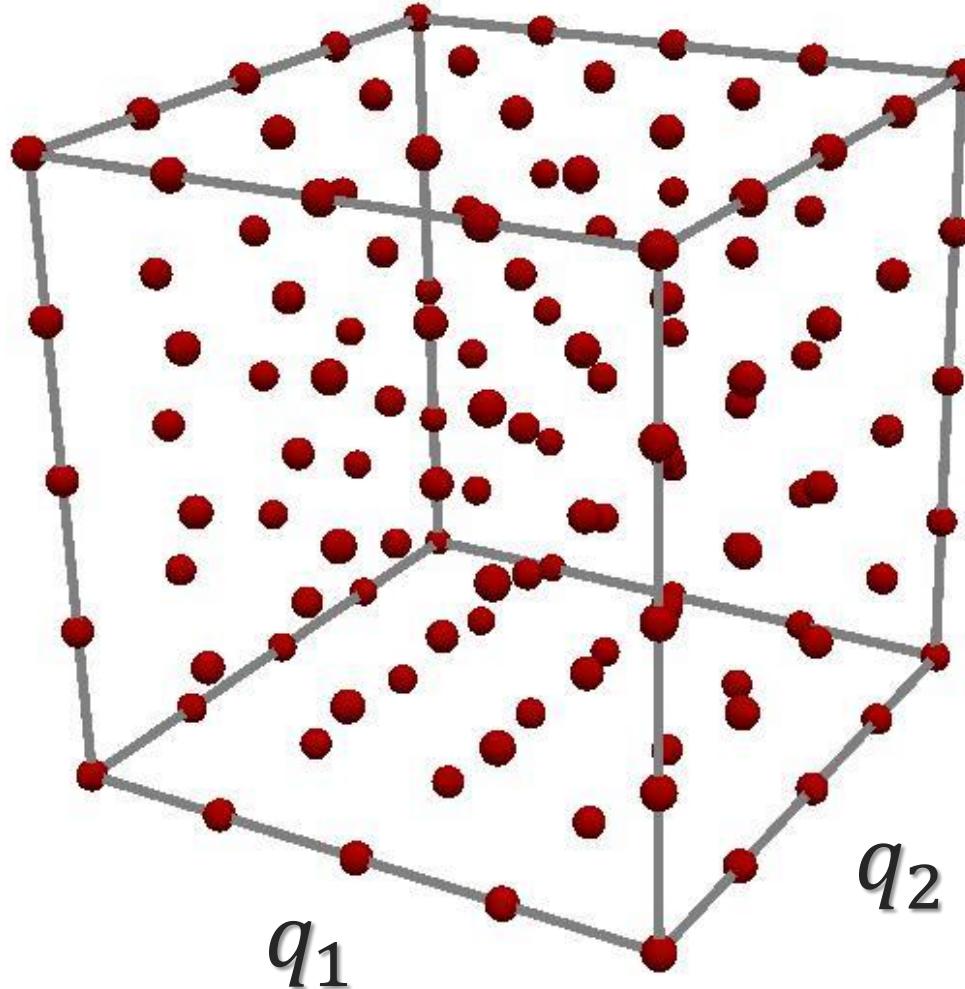
$$V = V(q_1, q_2, q_3)$$

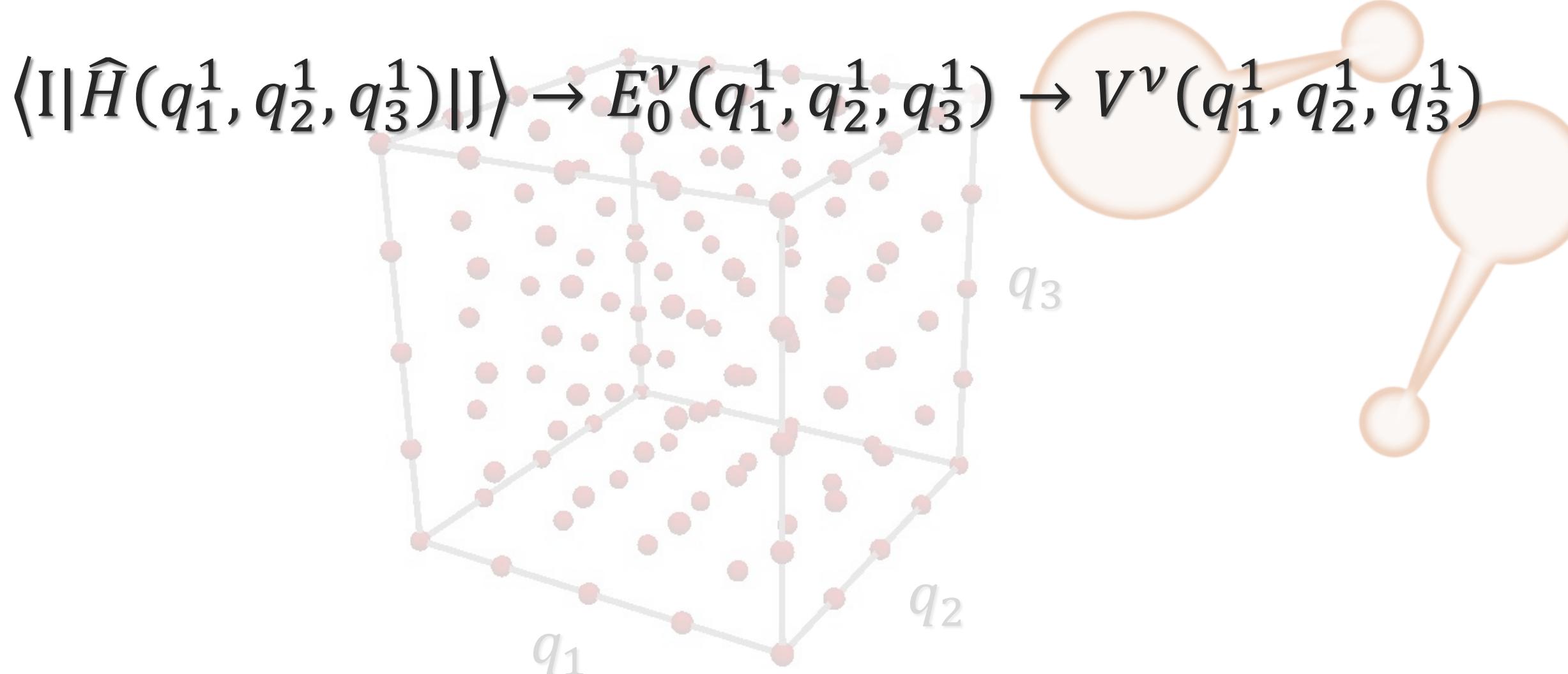


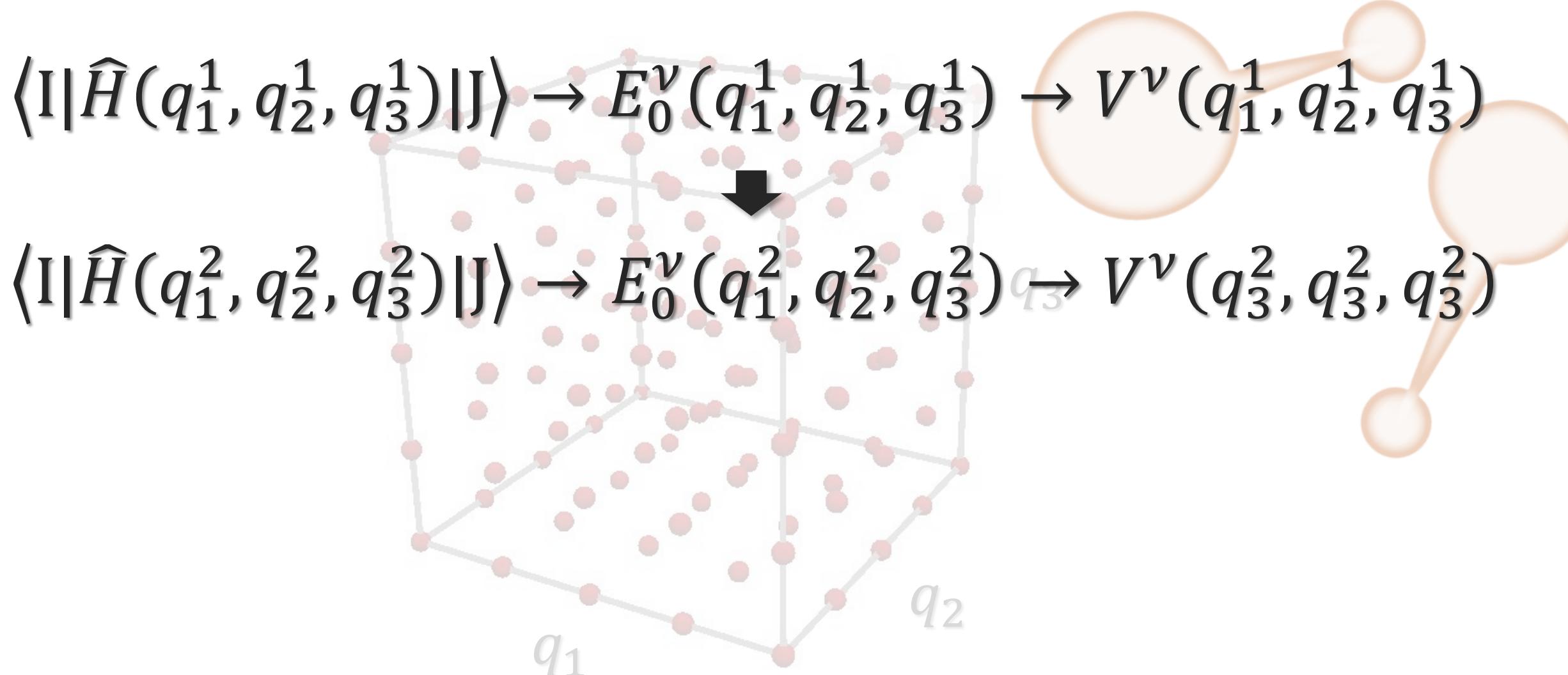


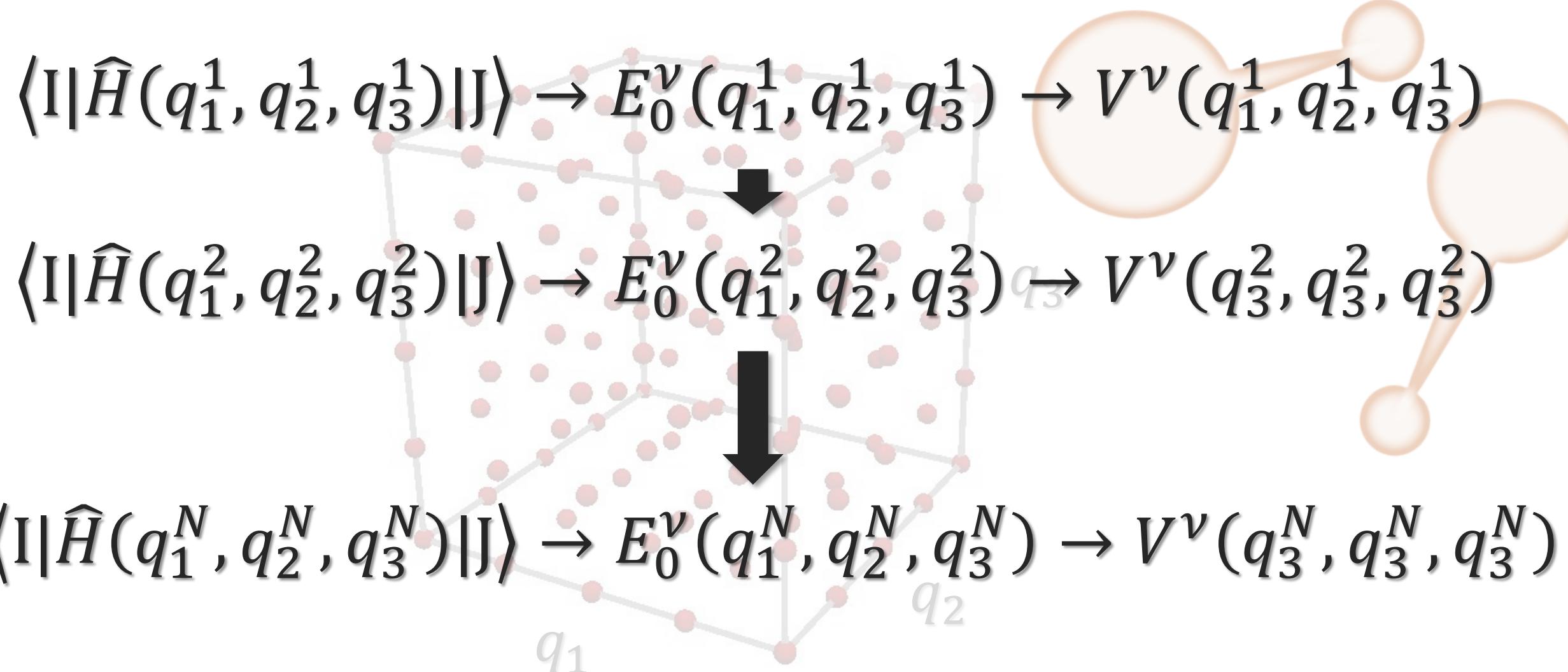






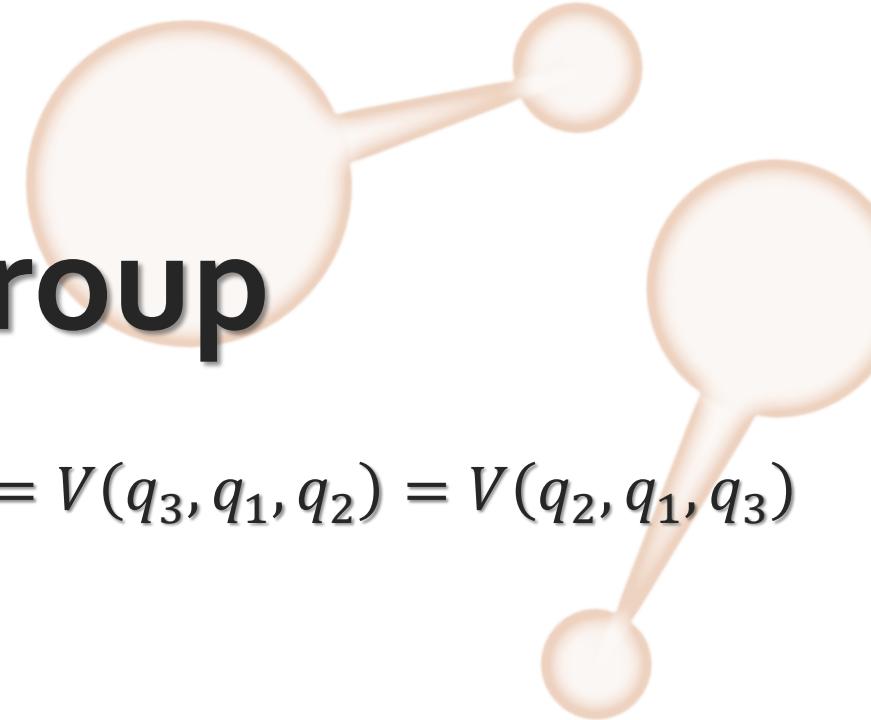








Symmetry Issues



S_3 Permutation Group

$$V(q_1, q_2, q_3) = V(q_2, q_1, q_3) = V(q_3, q_2, q_1) = V(q_1, q_3, q_2) = V(q_3, q_1, q_2) = V(q_2, q_1, q_3)$$

S_3 Permutation Group

$$V(q_1, q_2, q_3) = V(q_2, q_1, q_3) = V(q_3, q_2, q_1) = V(q_1, q_3, q_2) = V(q_3, q_1, q_2) = V(q_2, q_1, q_3)$$

P_{123}

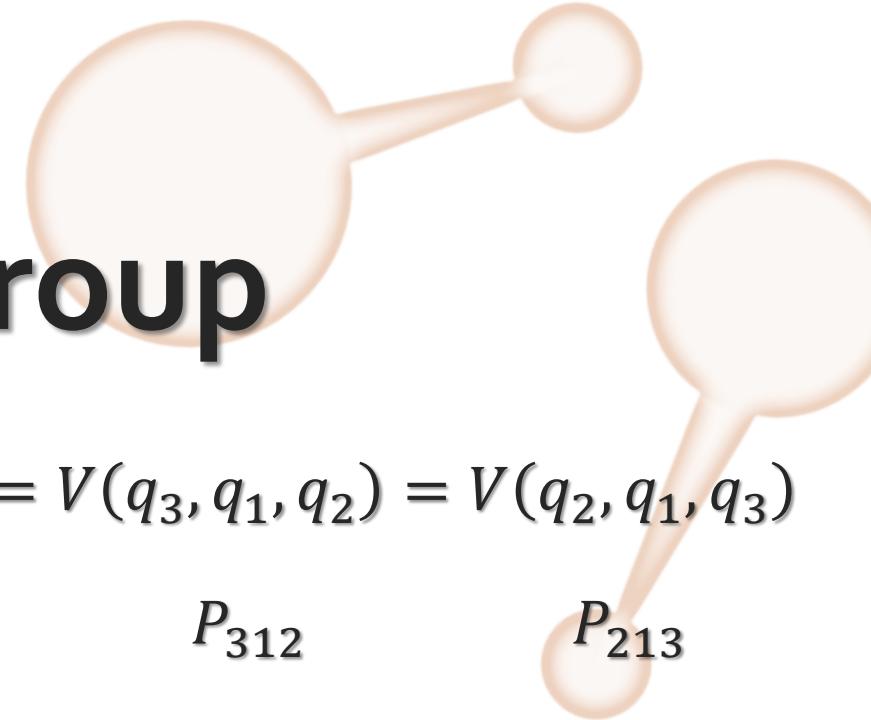
P_{213}

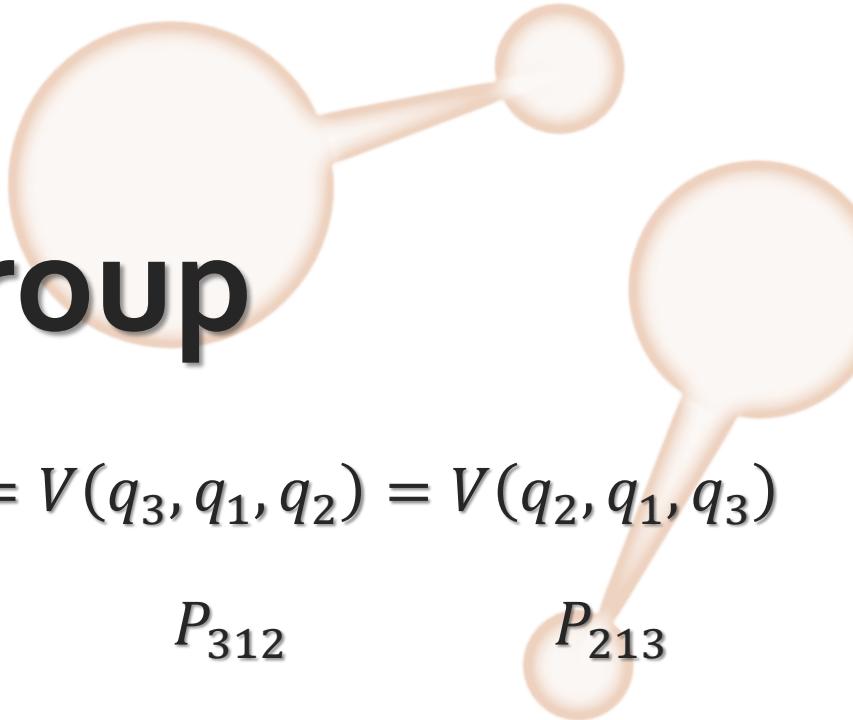
P_{321}

P_{132}

P_{312}

P_{213}





S_3 Permutation Group

$$V(q_1, q_2, q_3) = V(q_2, q_1, q_3) = V(q_3, q_2, q_1) = V(q_1, q_3, q_2) = V(q_3, q_1, q_2) = V(q_2, q_1, q_3)$$

P_{123}

P_{213}

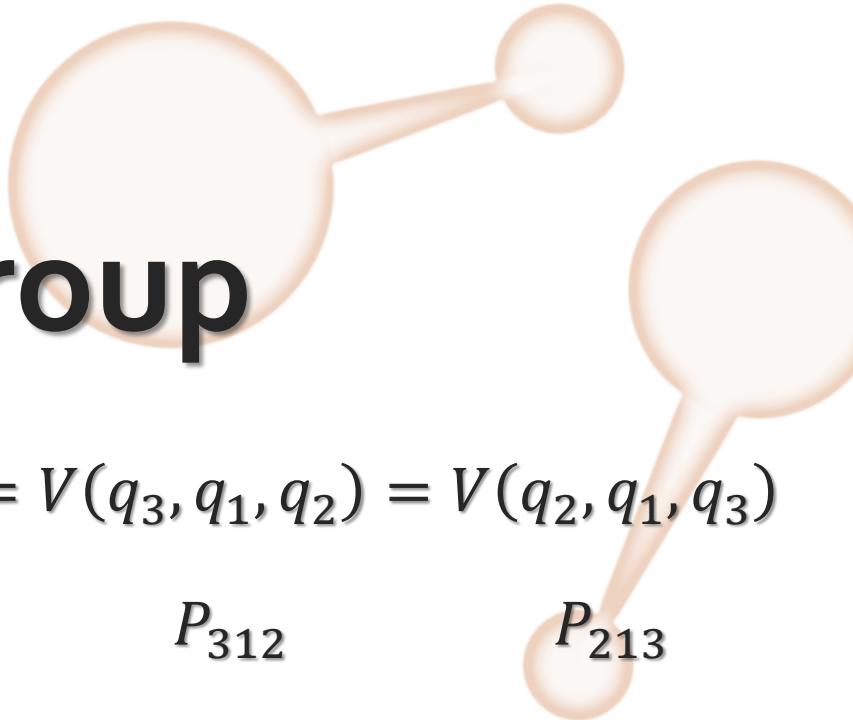
P_{321}

P_{132}

P_{312}

P_{213}

Identity



S_3 Permutation Group

$$V(q_1, q_2, q_3) = V(q_2, q_1, q_3) = V(q_3, q_2, q_1) = V(q_1, q_3, q_2) = V(q_3, q_1, q_2) = V(q_2, q_1, q_3)$$

P_{123}

P_{213}

P_{321}

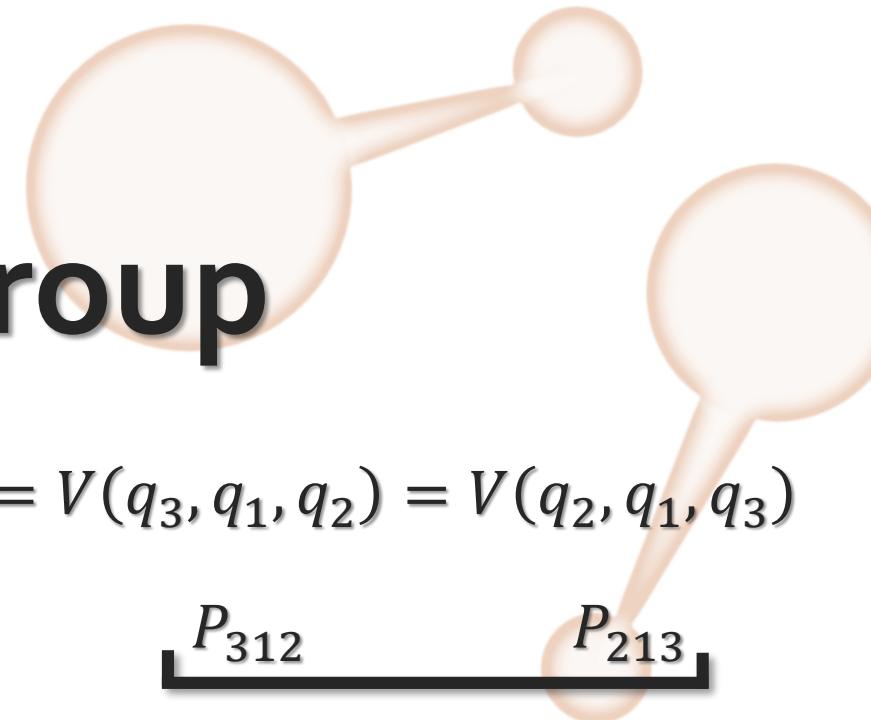
P_{132}

P_{312}

P_{213}

Identity

Exchange



S_3 Permutation Group

$$V(q_1, q_2, q_3) = V(q_2, q_1, q_3) = V(q_3, q_2, q_1) = V(q_1, q_3, q_2) = V(q_3, q_1, q_2) = V(q_2, q_1, q_3)$$

P_{123}

Identity

P_{213}

P_{321}

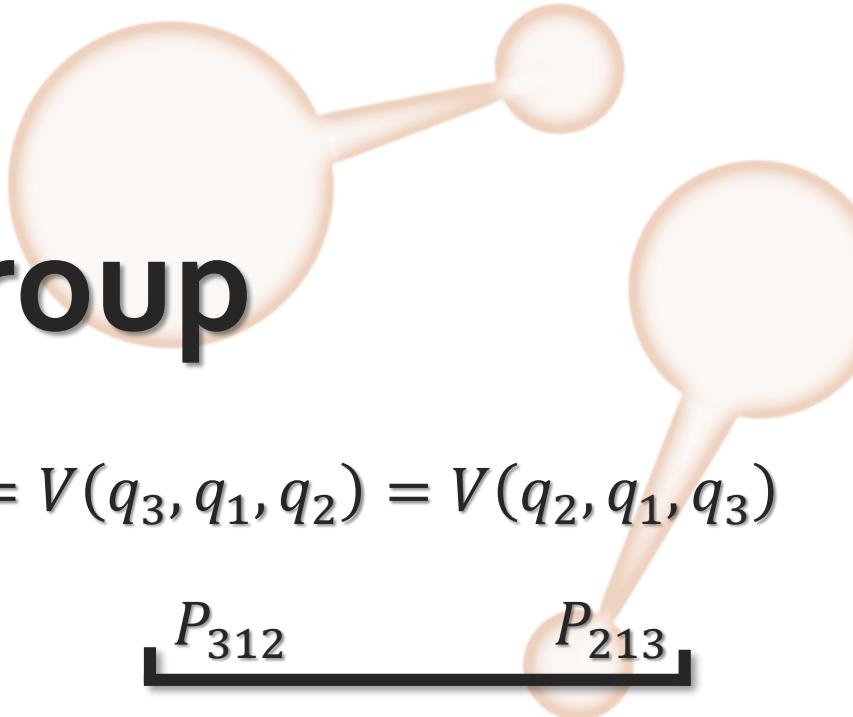
Exchange

P_{132}

P_{312}

P_{213}

Cyclic



S_3 Permutation Group

$$V(q_1, q_2, q_3) = V(q_2, q_1, q_3) = V(q_3, q_2, q_1) = V(q_1, q_3, q_2) = V(q_3, q_1, q_2) = V(q_2, q_1, q_3)$$

P_{123}

Identity

P_{213}

P_{321}

Exchange

P_{132}

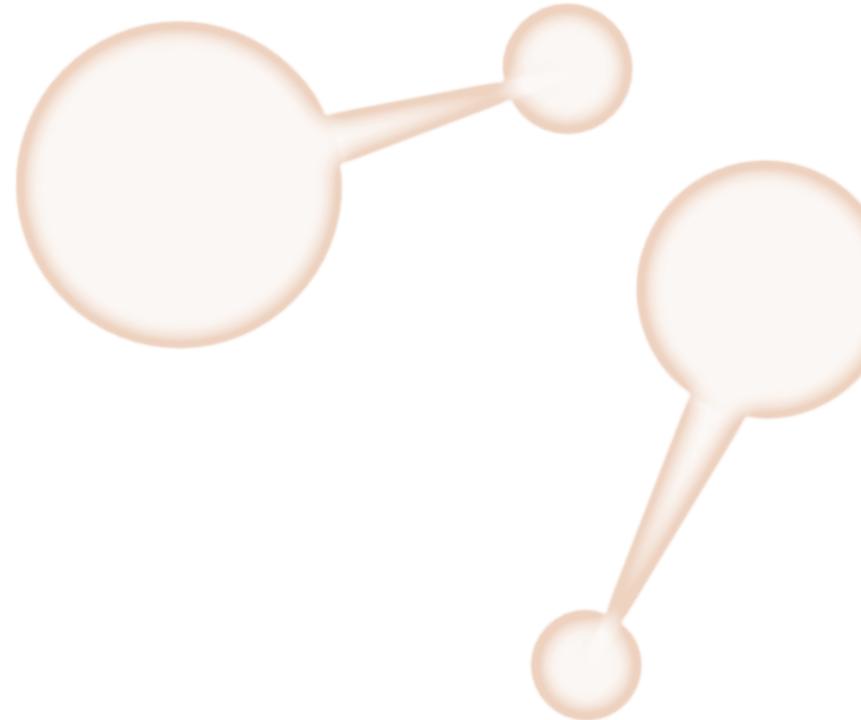
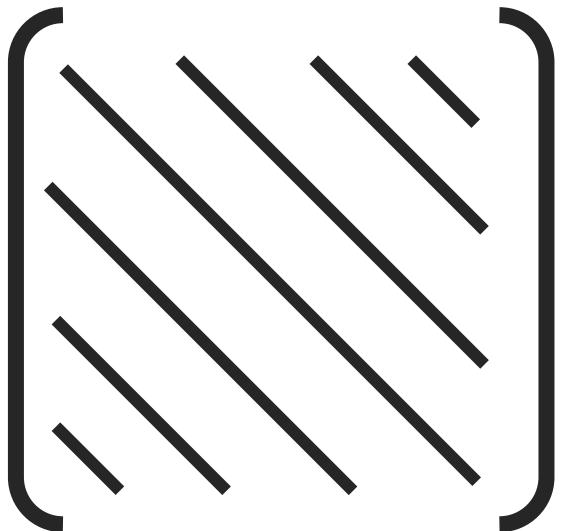
P_{312}

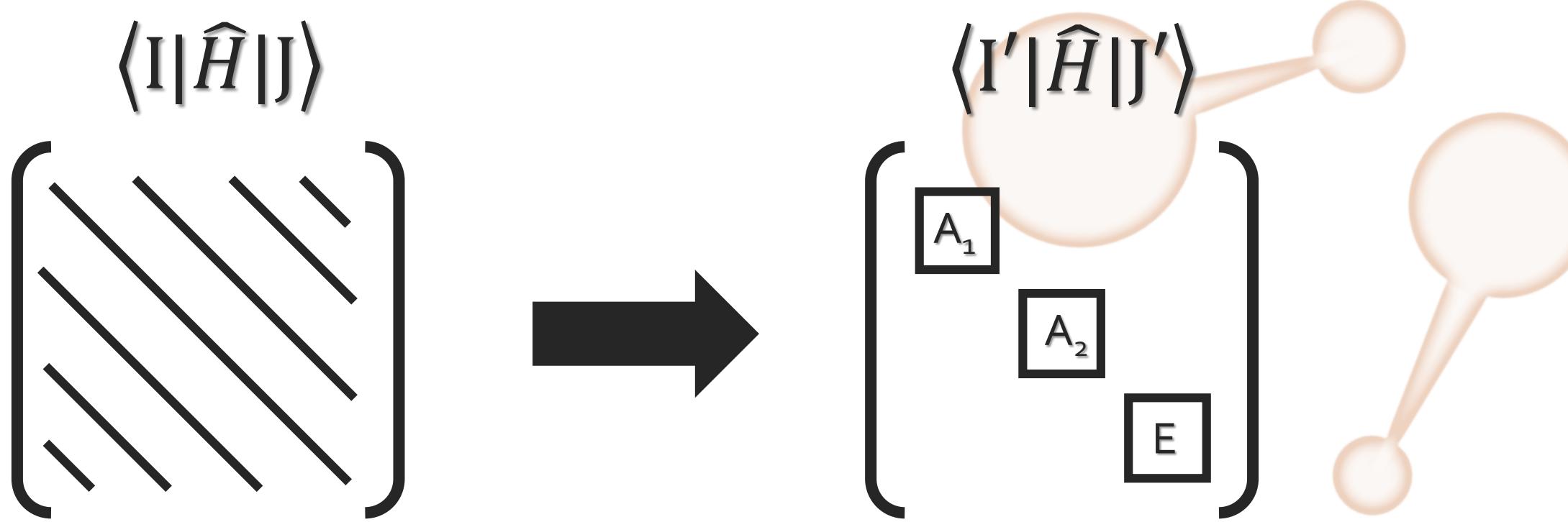
P_{213}

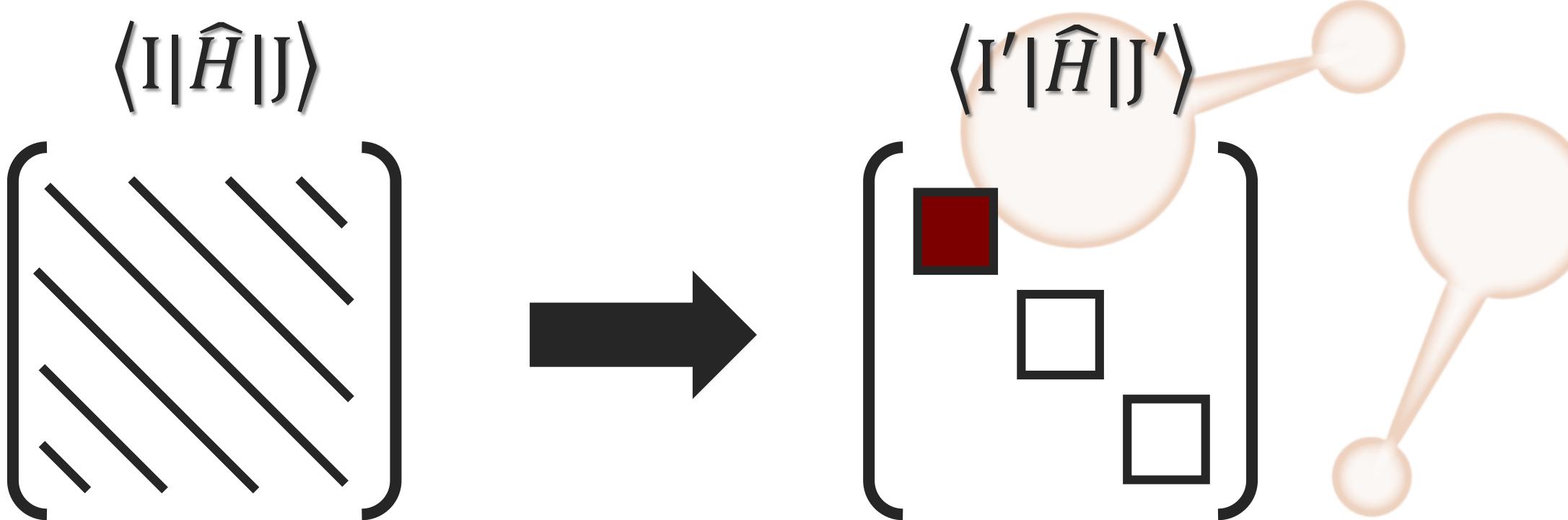
Cyclic

Example: $\hat{P}_{213}|l_1m_1\nu_1l_2m_2\nu_2l_3m_3\nu_3\rangle = |l_2m_2\nu_2l_1m_1\nu_1l_3m_3\nu_3\rangle$

$$\langle I | \hat{H} | J \rangle$$

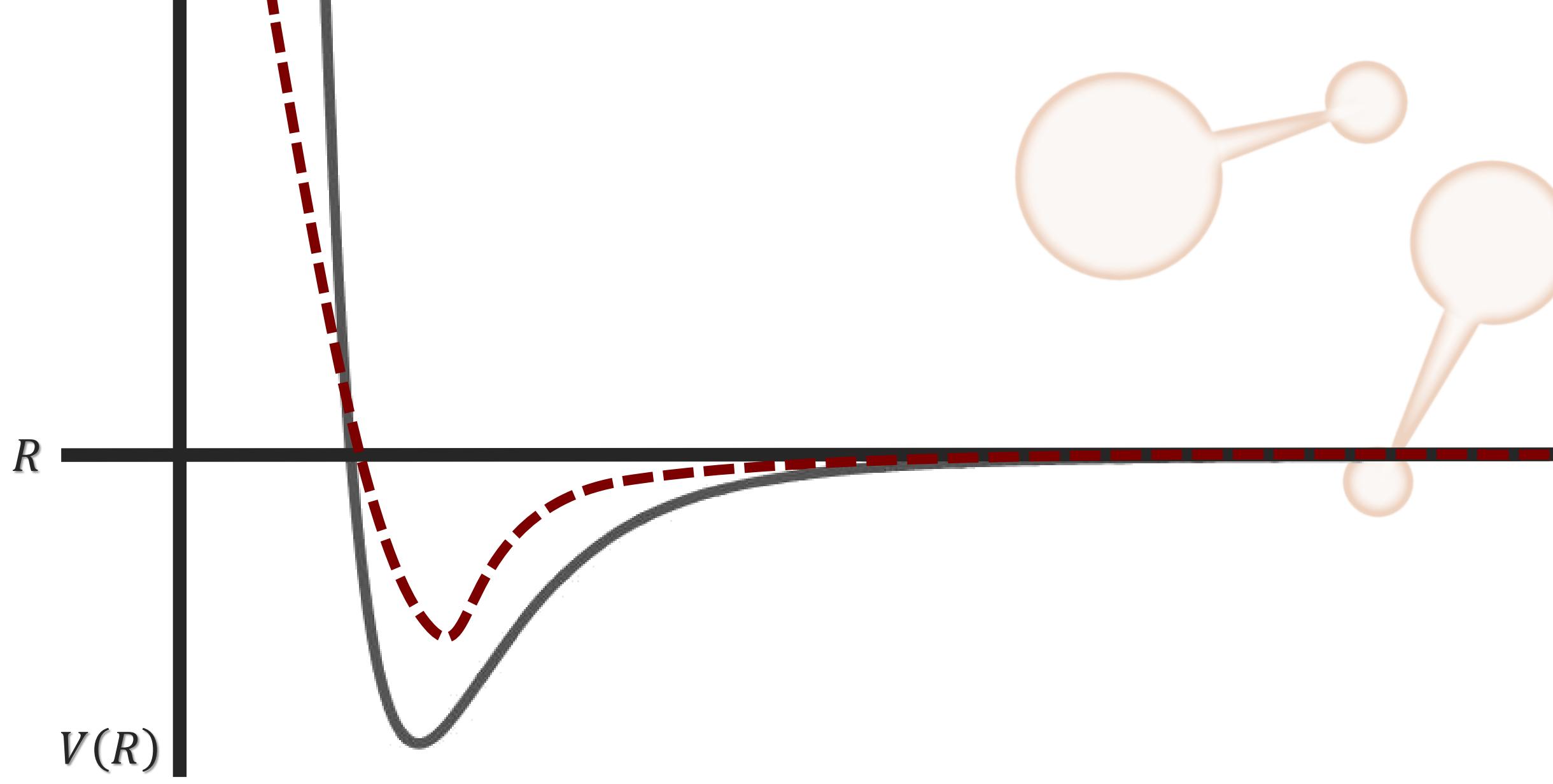






$$\hat{H}' = \hat{\Delta}_S \hat{H} \hat{\Delta}_S$$

$$\hat{\Delta}_S = \frac{1}{6} (P_{123} + P_{213} + P_{321} + P_{132} + P_{312} + P_{231})$$



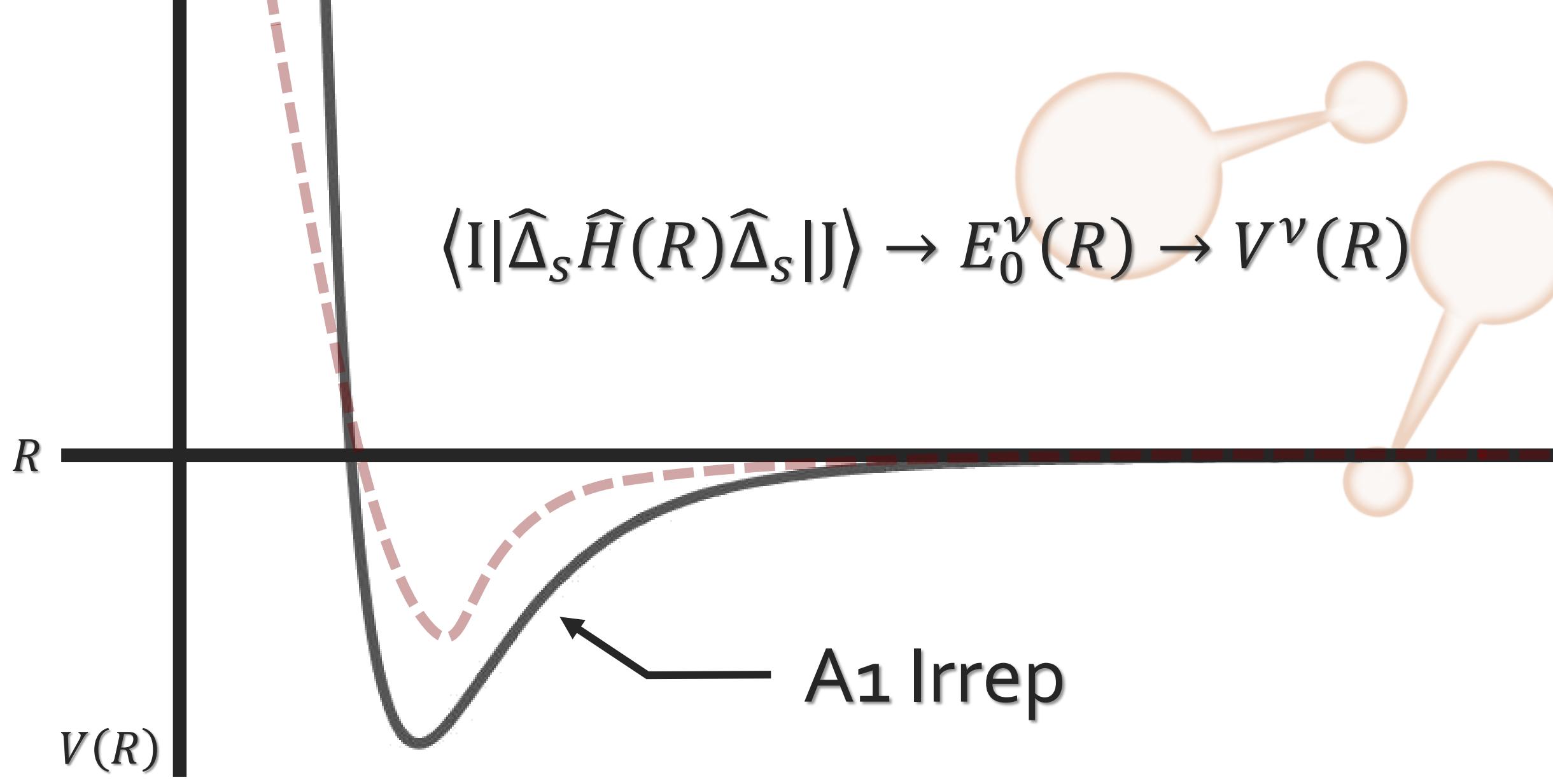
Conclusions

Confined Water

Dipole Chains

Hydrogen Clusters

Overview



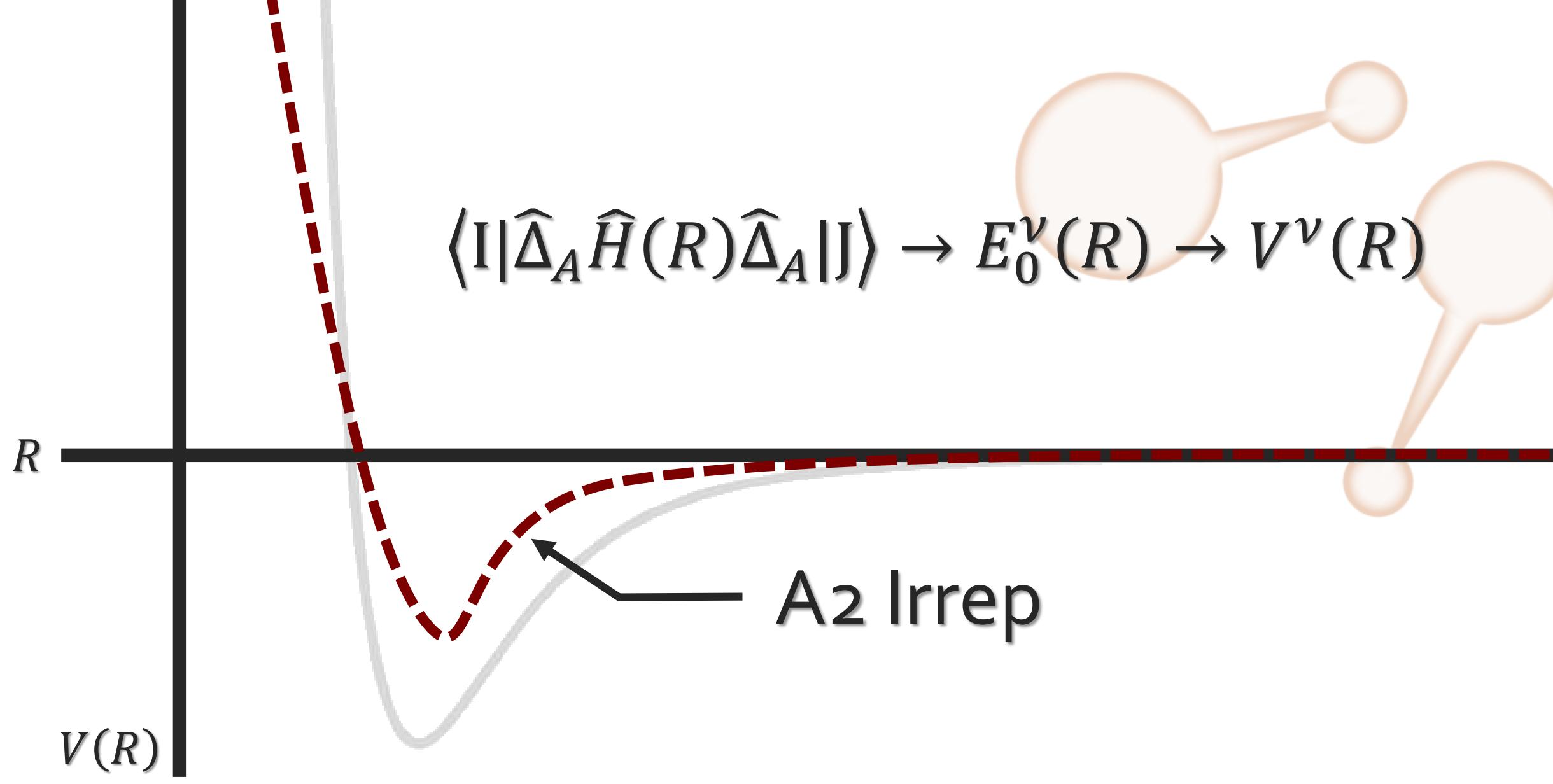
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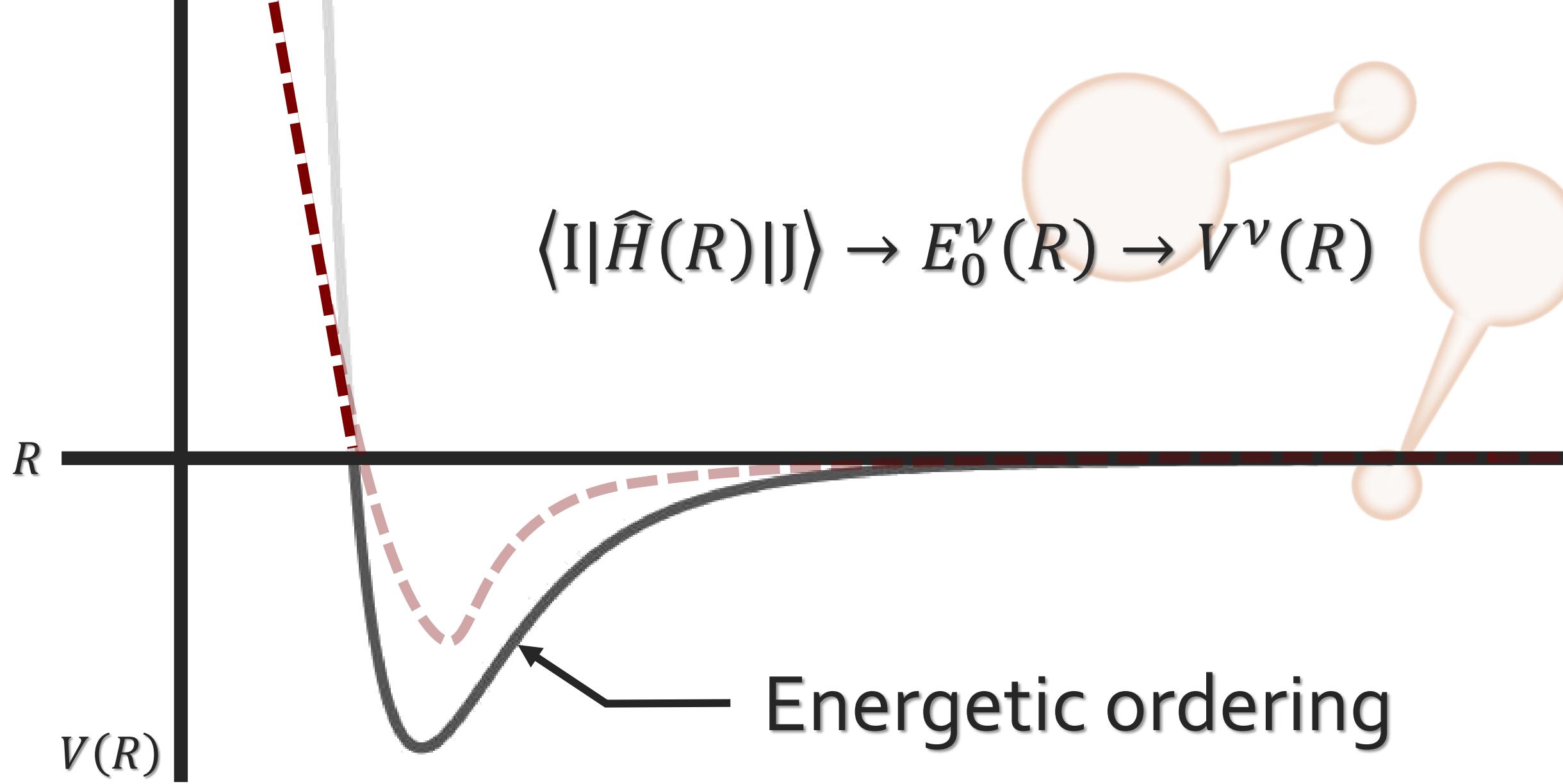
Conclusions

Confined Water

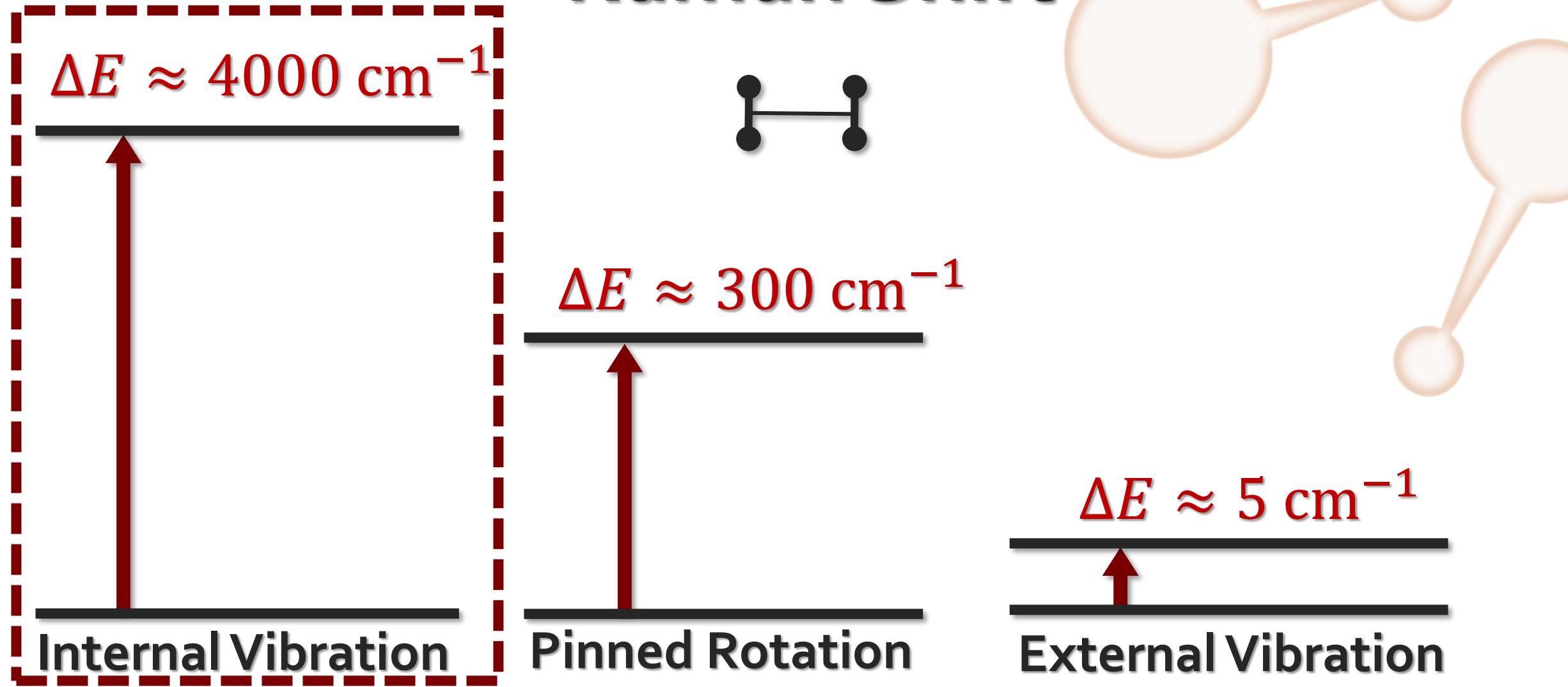
Dipole Chains

Hydrogen Clusters

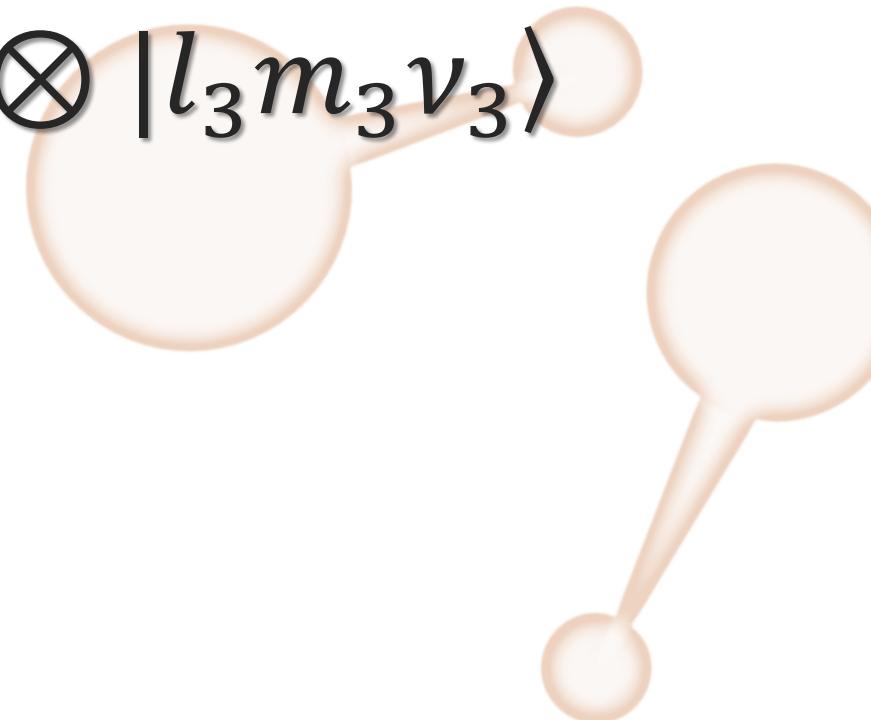
Overview



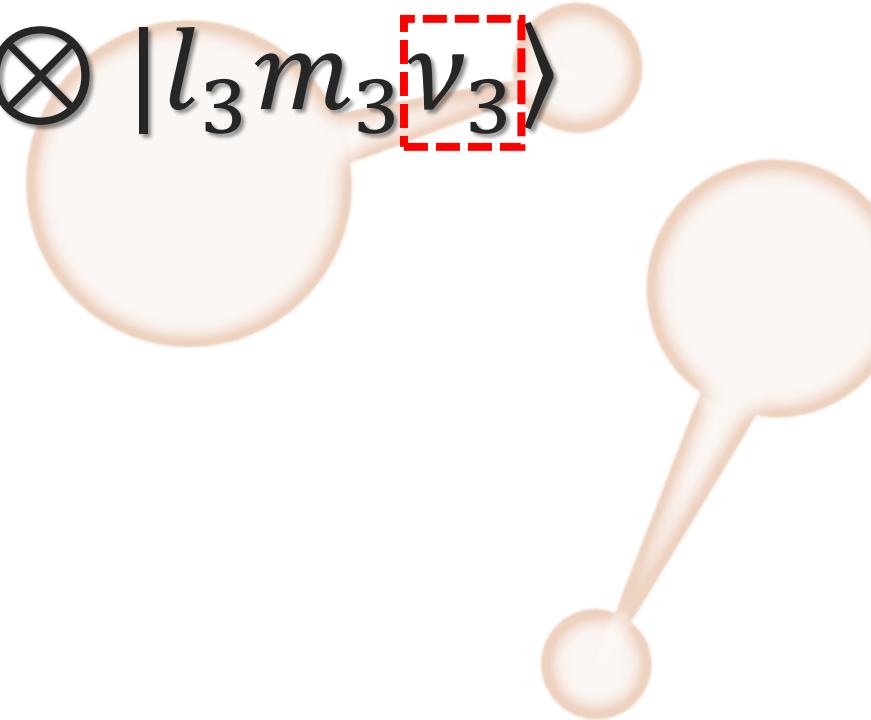
Raman Shift



$$|I\rangle = |l_1 m_1 \nu_1\rangle \otimes |l_2 m_2 \nu_2\rangle \otimes |l_3 m_3 \nu_3\rangle$$



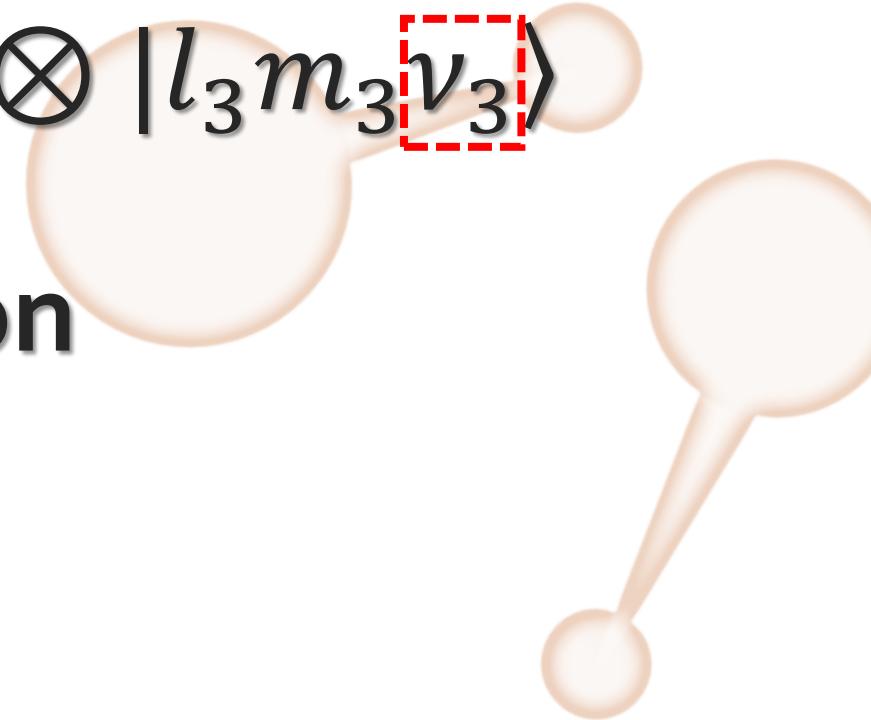
$$|I\rangle = |l_1 m_1 [v_1]\rangle \otimes |l_2 m_2 [v_2]\rangle \otimes |l_3 m_3 [v_3]\rangle$$



$$|I\rangle = |l_1 m_1 \nu_1\rangle \otimes |l_2 m_2 \nu_2\rangle \otimes |l_3 m_3 \nu_3\rangle$$

Adiabatic Truncation

$$\sum_{i=1}^3 \nu_i = \nu$$



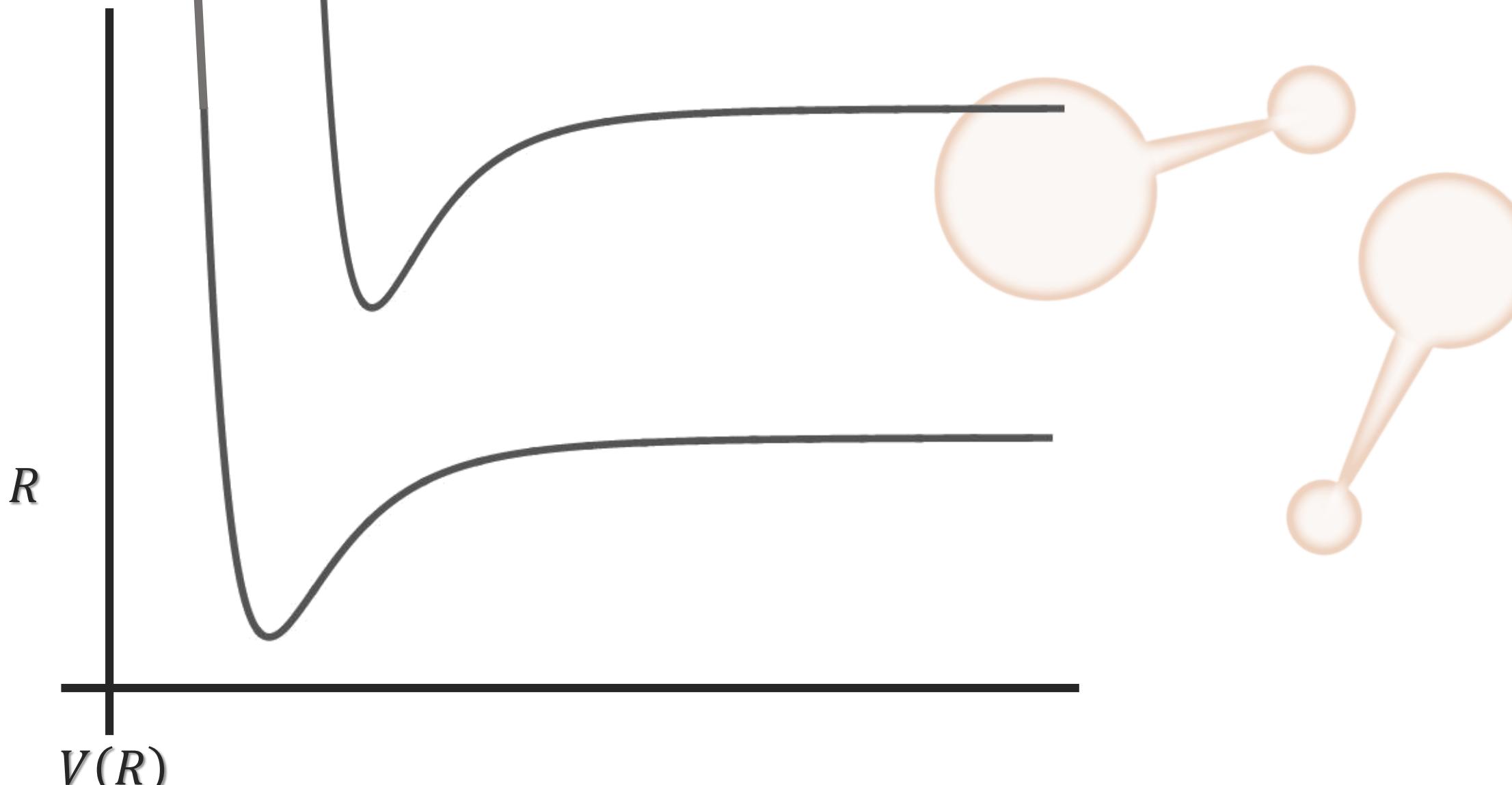
$$|I\rangle = |l_1 m_1 \nu_1\rangle \otimes |l_2 m_2 \nu_2\rangle \otimes |l_3 m_3 \nu_3\rangle$$

Adiabatic Truncation

$$\sum_{i=1}^3 \nu_i = \nu$$



Ground Surface: $\nu = 0$
Excited Surface: $\nu = 1$



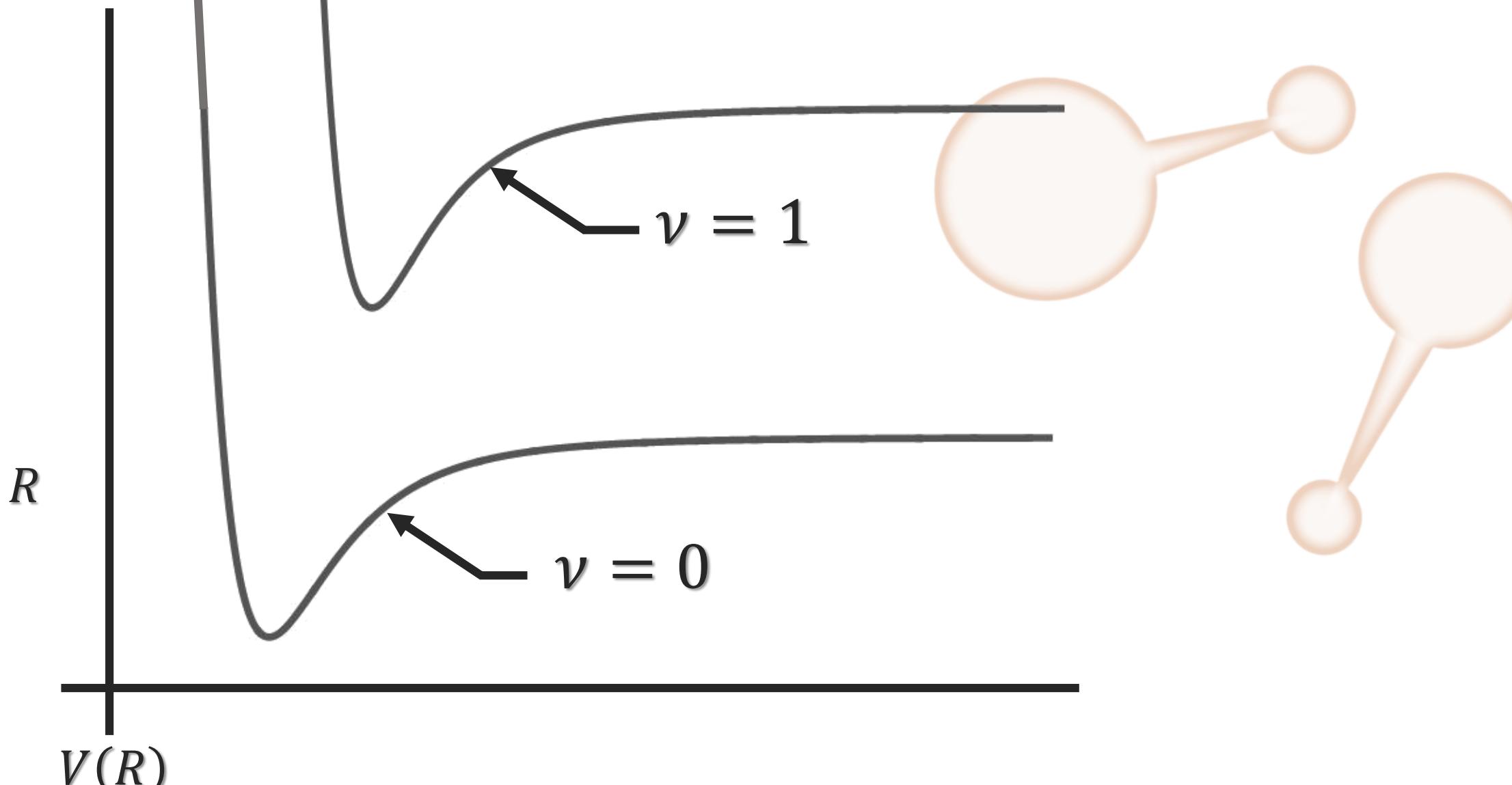
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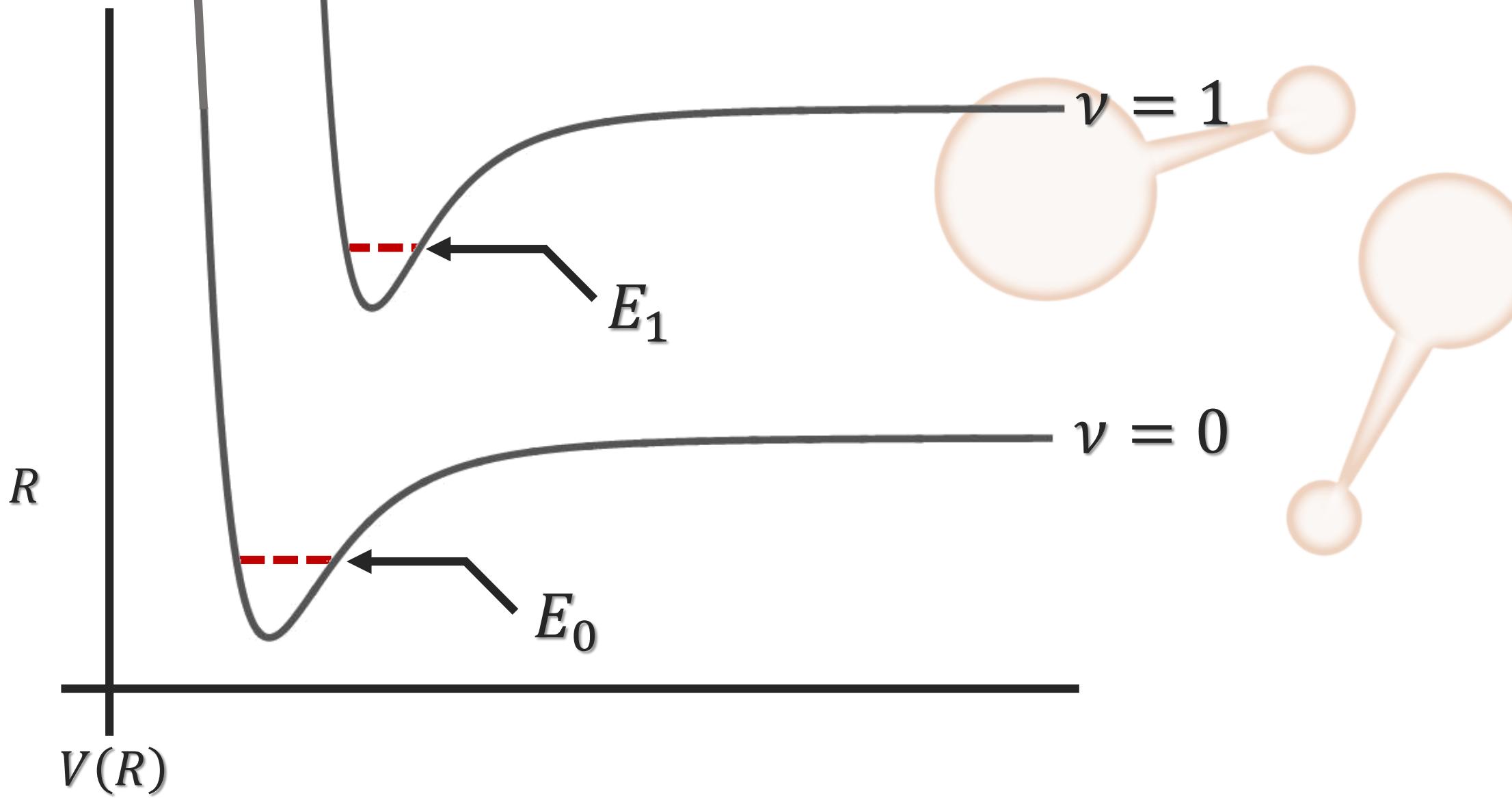
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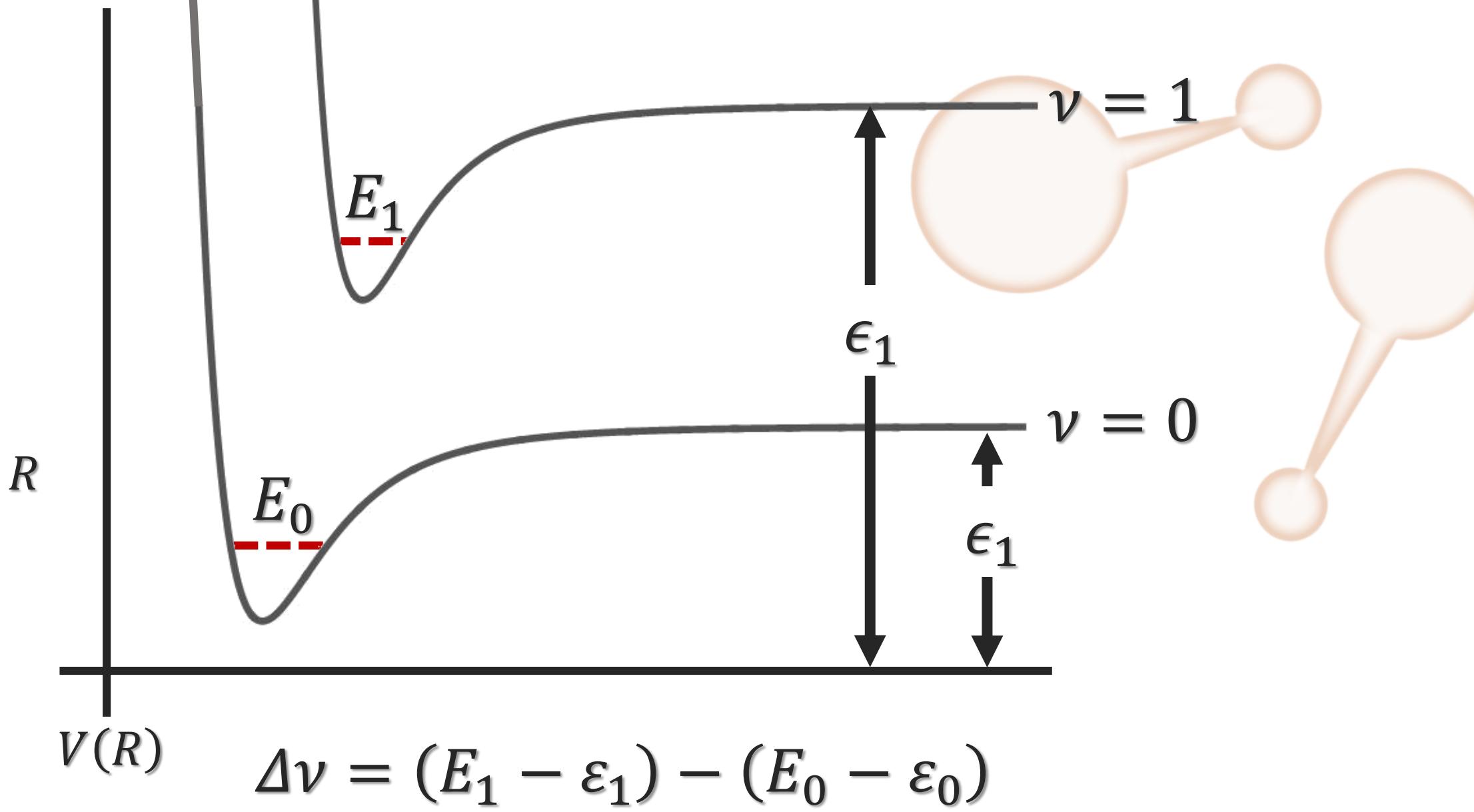
Conclusions

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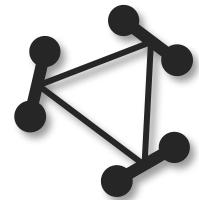
Conclusions

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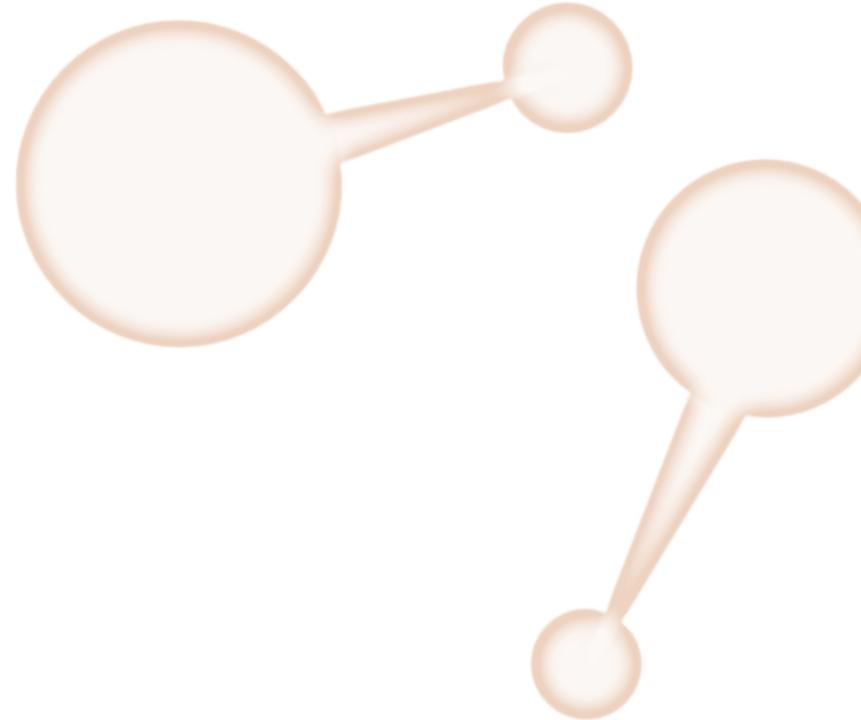
Overview

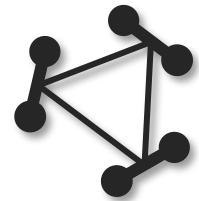


Many Body



Pairwise Additive





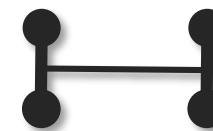
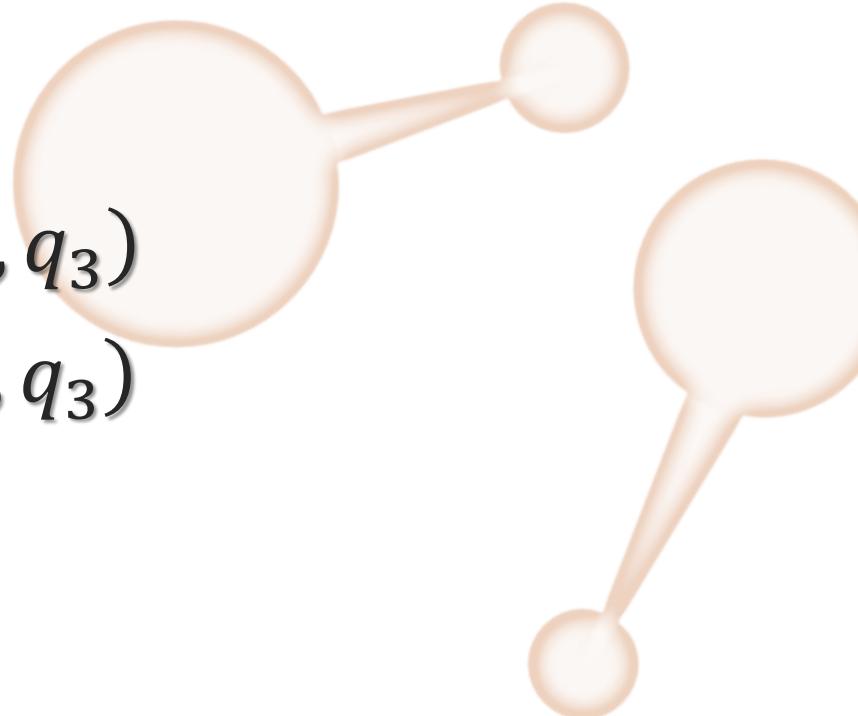
Many Body

Ground Surface:

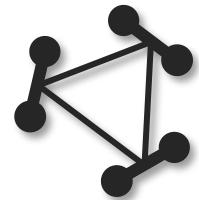
$$V^0 = V^0(q_1, q_2, q_3)$$

Excited Surface:

$$V^1 = V^1(q_1, q_2, q_3)$$



Pairwise Additive



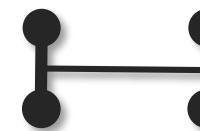
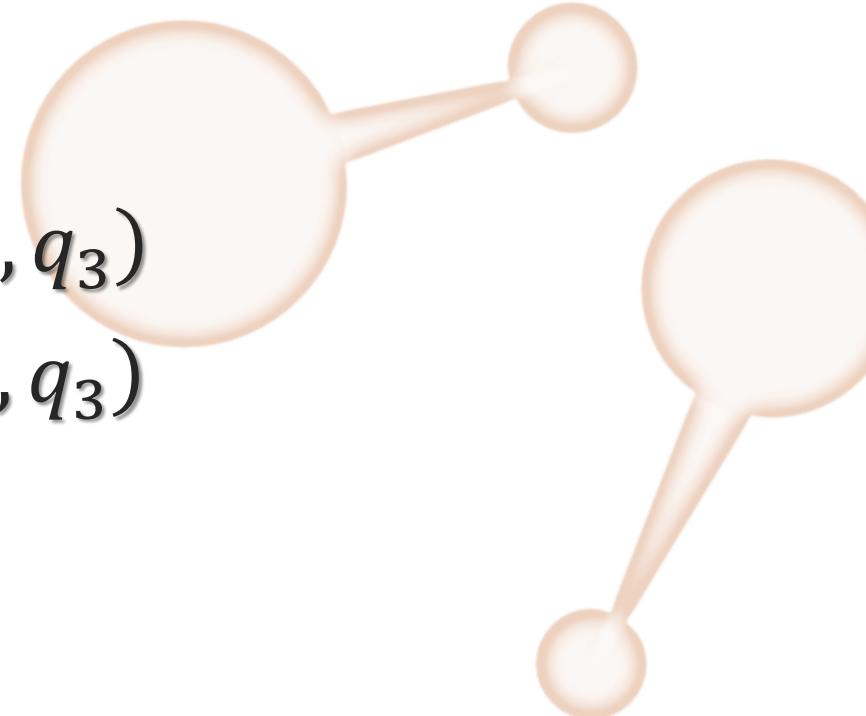
Many Body

Ground Surface:

$$V^0 = V^0(q_1, q_2, q_3)$$

Excited Surface:

$$V^1 = V^1(q_1, q_2, q_3)$$



Pairwise Additive

Ground Surface:

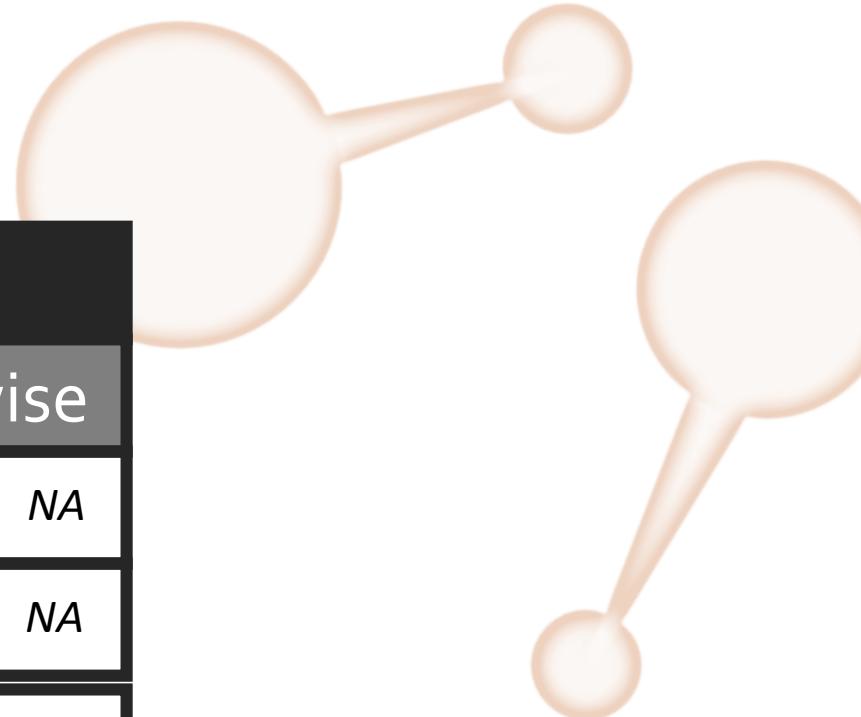
$$V^0(q_1, q_2, q_3) = \sum_{i < j} V^0(q_i, q_j)$$

Excited Surface:

$$V^1(q_1, q_2, q_3) = \frac{1}{3} \sum_{i < j} V^0(q_i, q_j) + \frac{2}{3} \sum_{i < j} V^1(q_i, q_j)$$

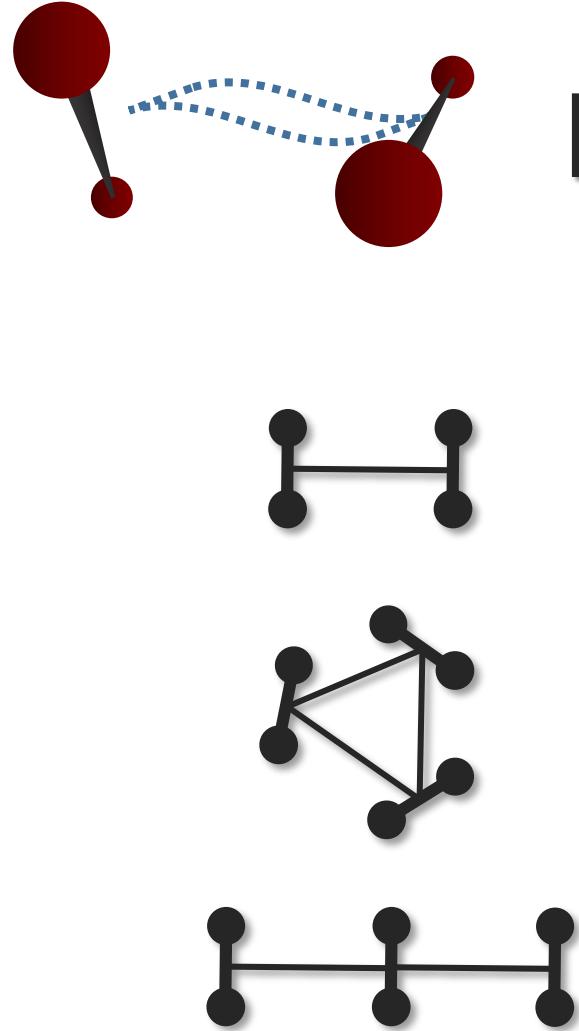
Hydrogen Trimer

mass = 2.015650642 amu



State Label	Energy (cm ⁻¹)	
	Many Body	Pairwise
$E_0^0 - \epsilon^0$	-9.8626	NA
$E_1^0 - \epsilon^0$	-3.6316	NA
$E_0^1 - \epsilon^1$	-10.6839	NA
$E_0^1 - \epsilon^1$	-4.1110	NA
$\Delta\nu$	-0.821 (-0.822)	-0.825

Vibrational Entanglement



$\nu = 0$

0.999

0.999

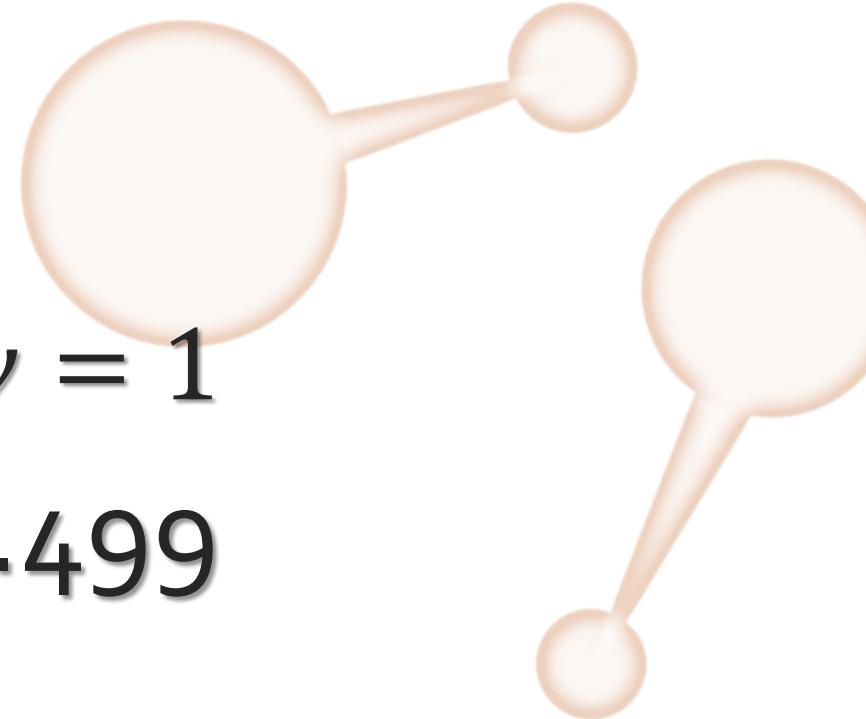
0.999

$\nu = 1$

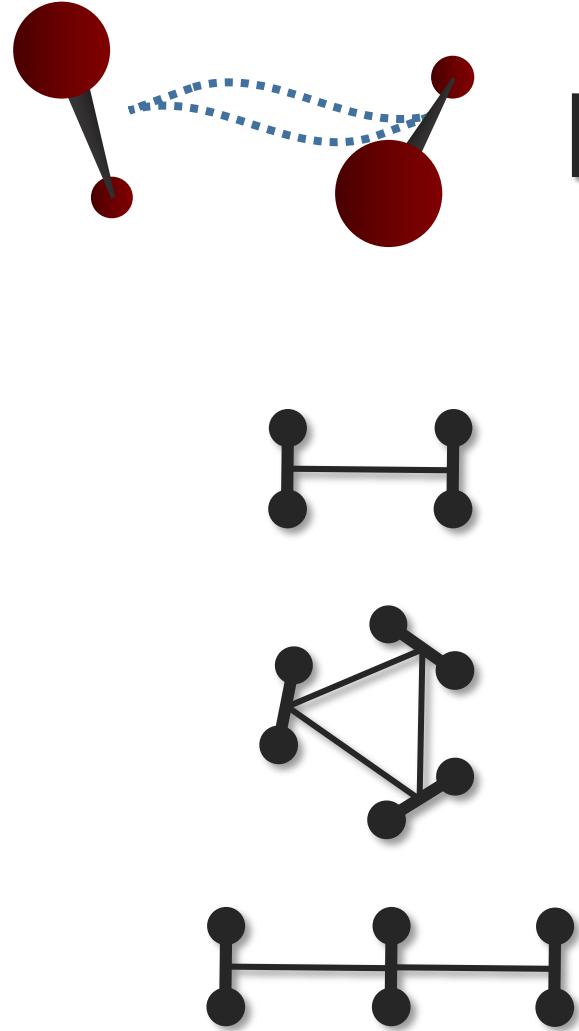
0.499

0.554

0.556



Vibrational Entanglement

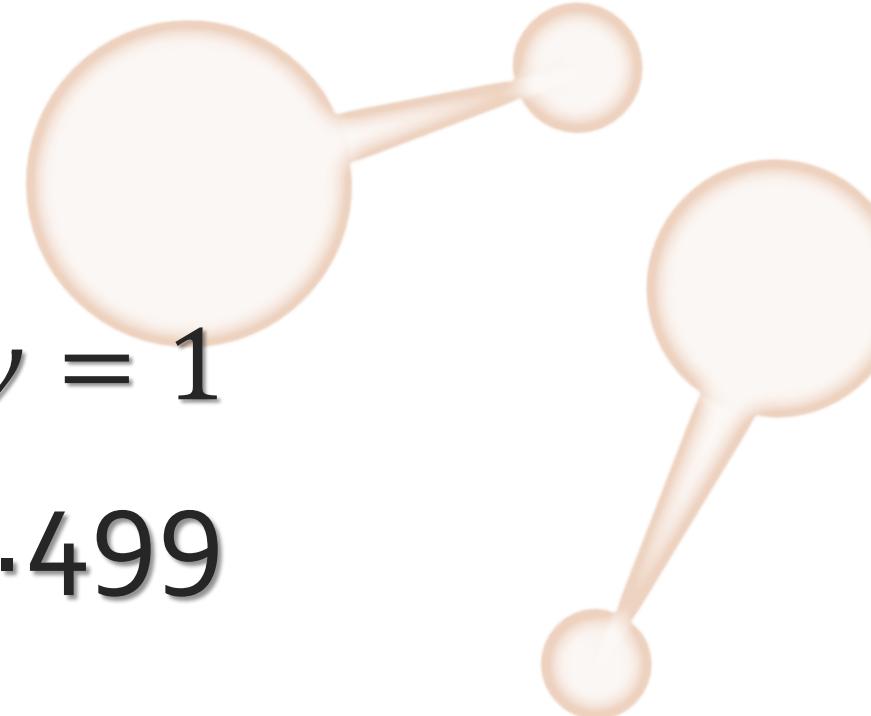


$\nu = 0$

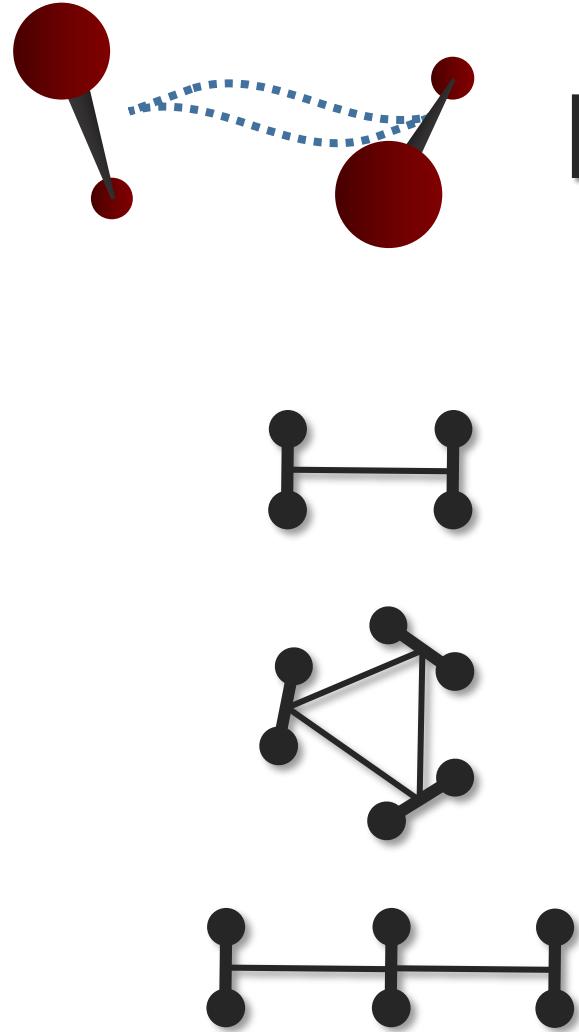
0.999
0.999
0.999

$\nu = 1$

0.499
0.554
0.556



Vibrational Entanglement



$\nu = 0$

0.999

0.999

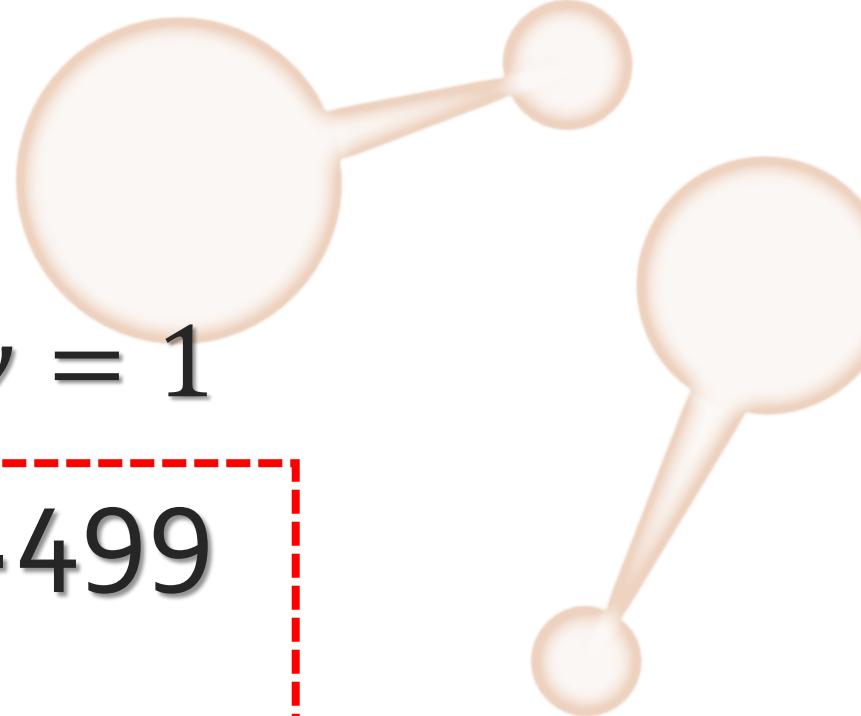
0.999

$\nu = 1$

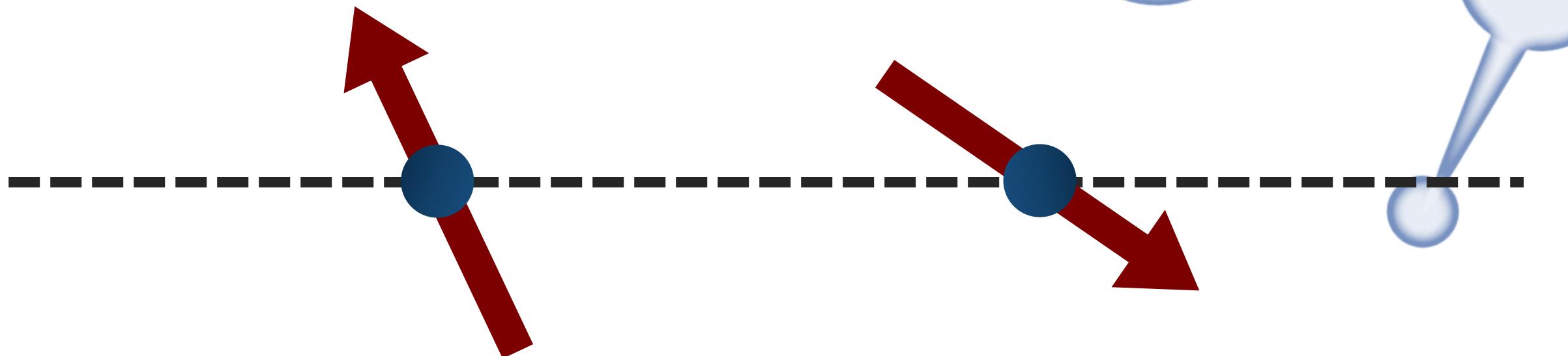
0.499

0.554

0.556



Dipole Chains



$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j-i)^3}$$

$$\langle I | \hat{H} | J \rangle \Rightarrow \{ |\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle, \dots \}$$

$$|I\rangle = \prod_{i=1}^N |l_i m_i\rangle$$

$$\hat{l}^2 |lm\rangle = l(l+1) |lm\rangle$$

$$\hat{L}_z |lm\rangle = m^2 |lm\rangle$$



$$H = \boxed{\alpha} \sum_{i=1}^N \hat{l}_i^2 + \boxed{\frac{\beta}{d^3}} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j-i)^3}$$

$$\langle I | \hat{H} | J \rangle \Rightarrow \{ |\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle, \dots \}$$

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$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j-i)^3}$$

$$\langle I | \hat{H} | J \rangle \Rightarrow \{ |\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle, \dots \}$$

$$|I\rangle = \prod_{i=1}^N |l_i m_i\rangle$$

$$\hat{l}^2 |lm\rangle = l(l+1) |lm\rangle$$

$$\hat{L}_z |lm\rangle = m^2 |lm\rangle$$



$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j-i)^3}$$

$$\langle I | \hat{H} | J \rangle \Rightarrow \{ |\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle, \dots \}$$

$$|I\rangle = \prod_{i=1}^N |l_i m_i\rangle$$

$$\hat{l}^2 |lm\rangle = l(l+1) |lm\rangle$$

$$l_z |lm\rangle = m^2 |lm\rangle$$



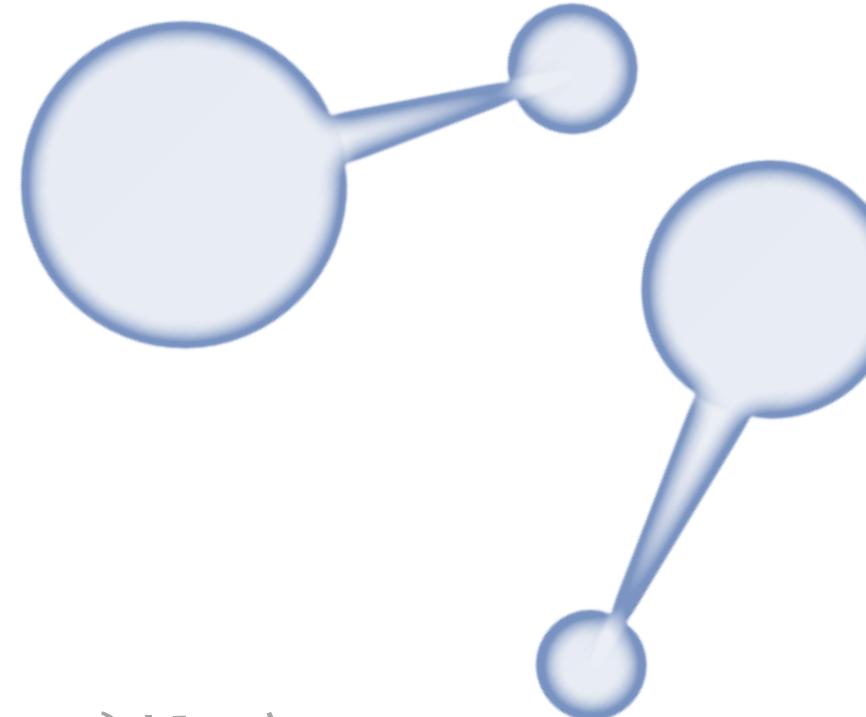
Polyad Truncation

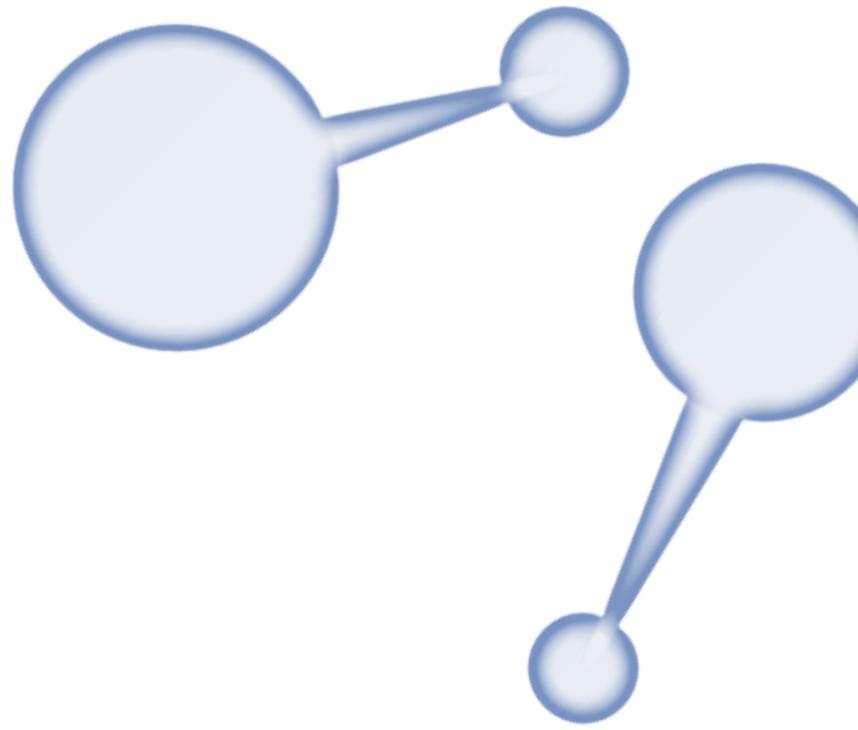
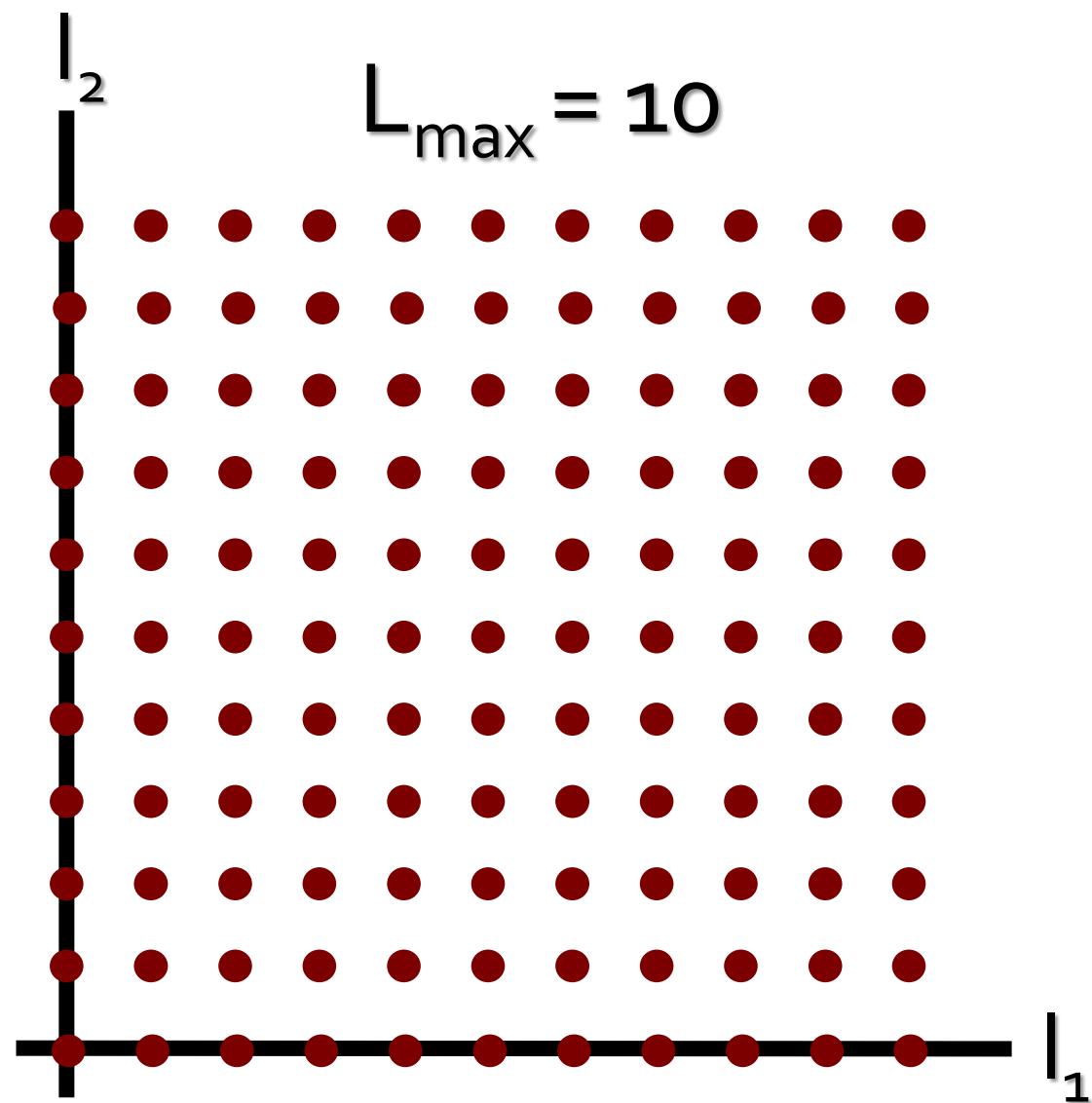
$$\sum_{i=1}^N l_i \leq L_{\max}$$

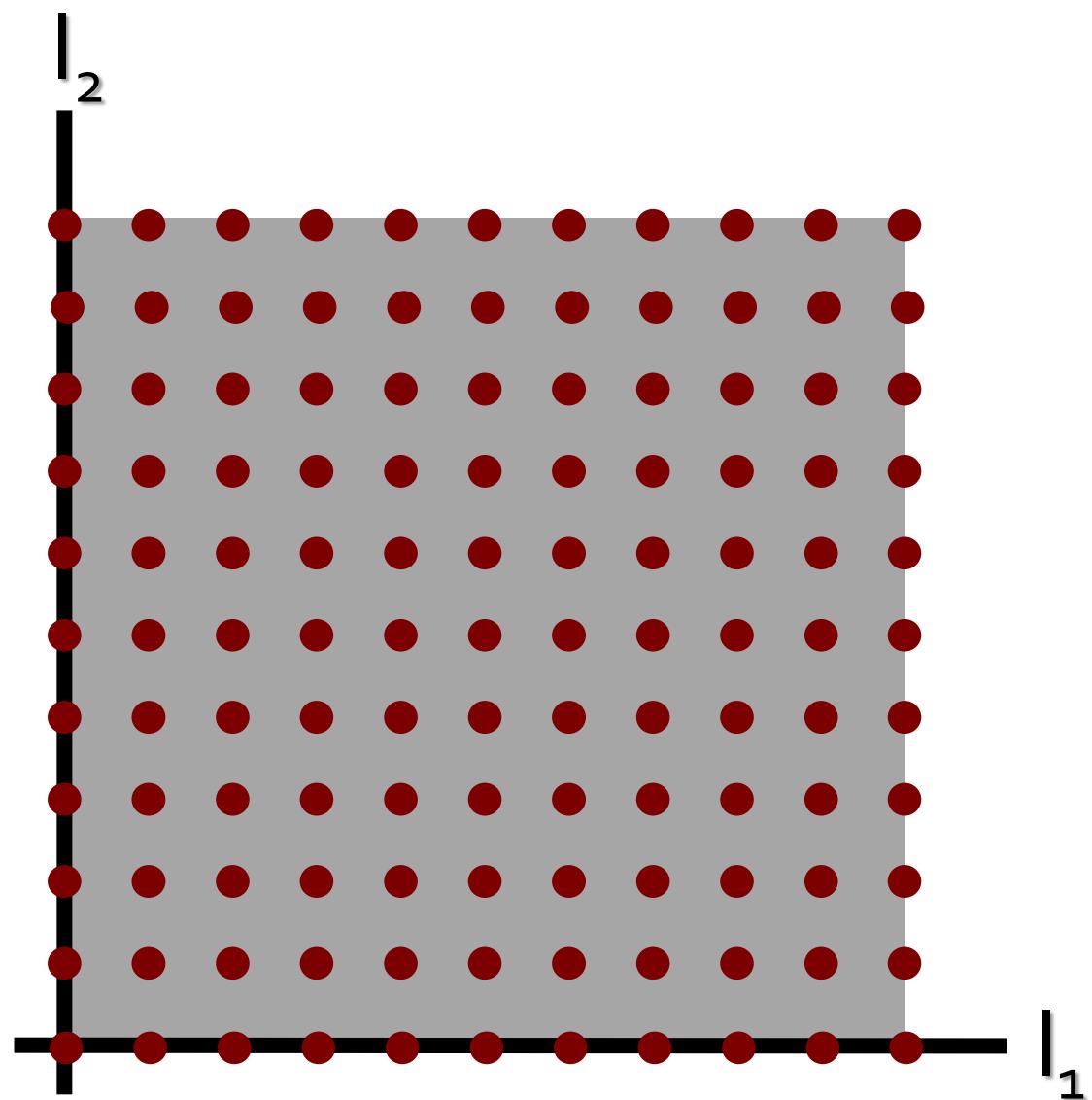
$$|I\rangle = \prod_{i=1}^N |l_i m_i\rangle$$

$$\hat{l}^2 |lm\rangle = l(l+1) |lm\rangle$$

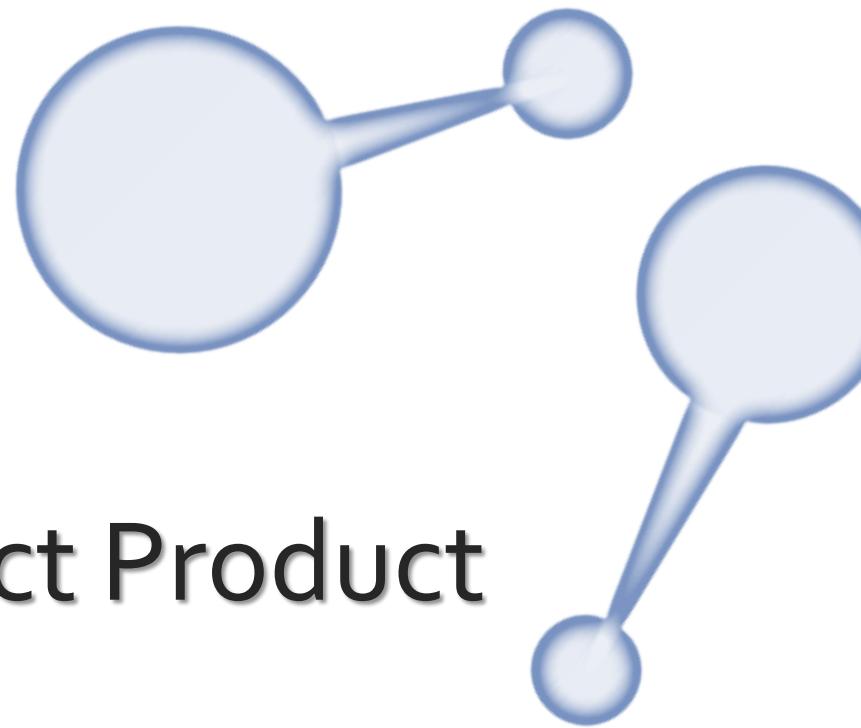
$$l_z |lm\rangle = m^2 |lm\rangle$$

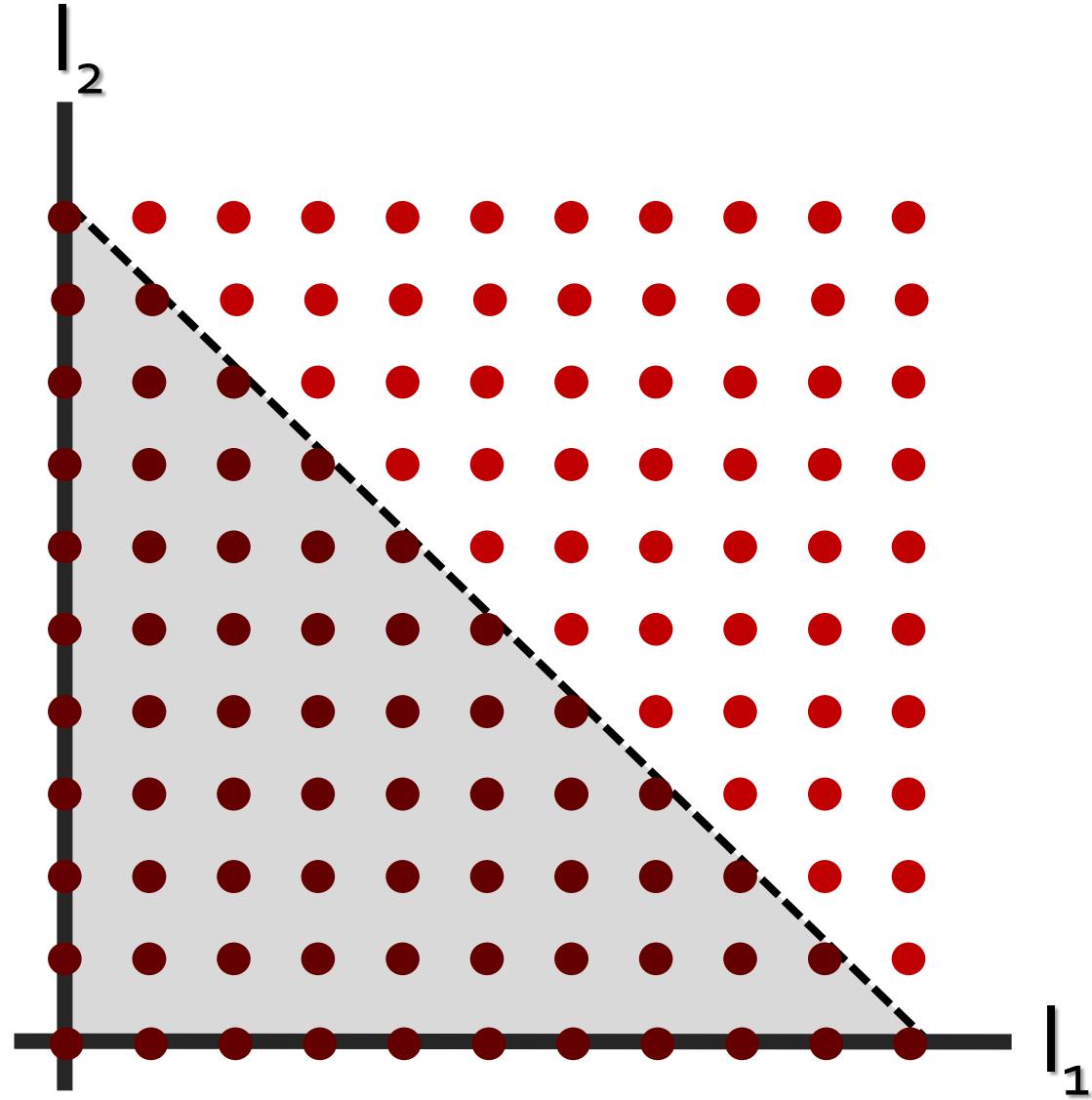




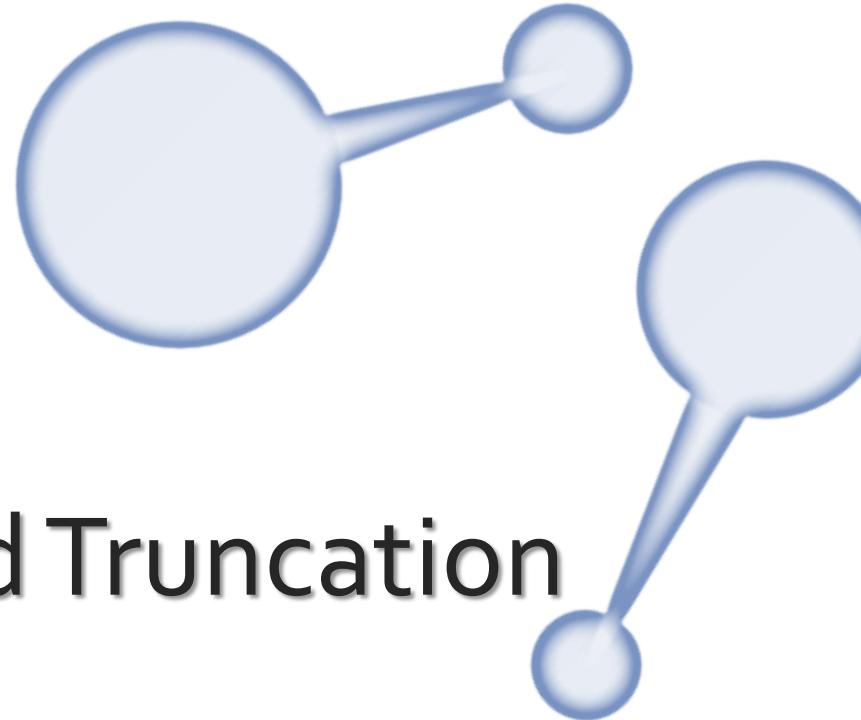


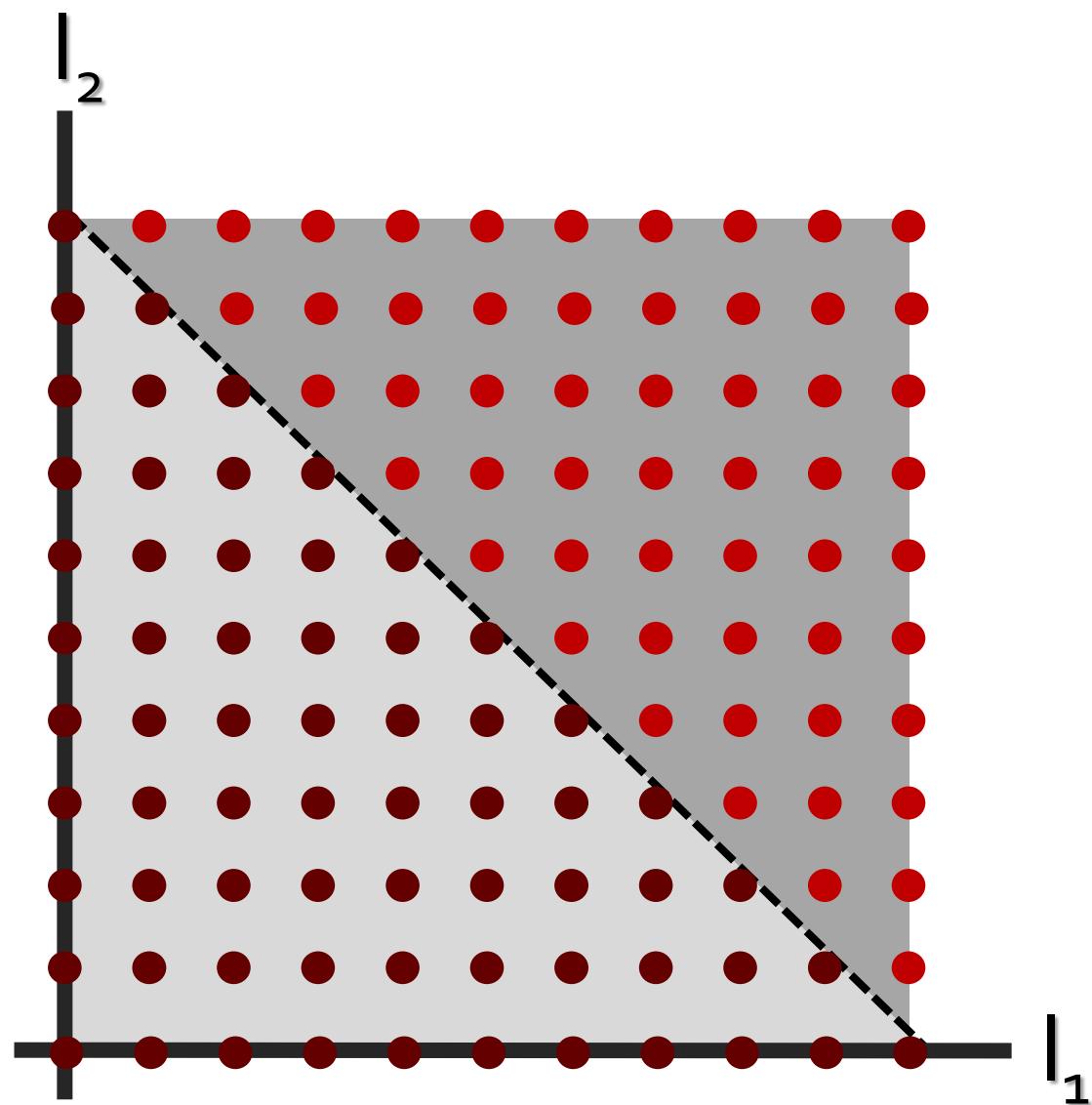
Direct Product



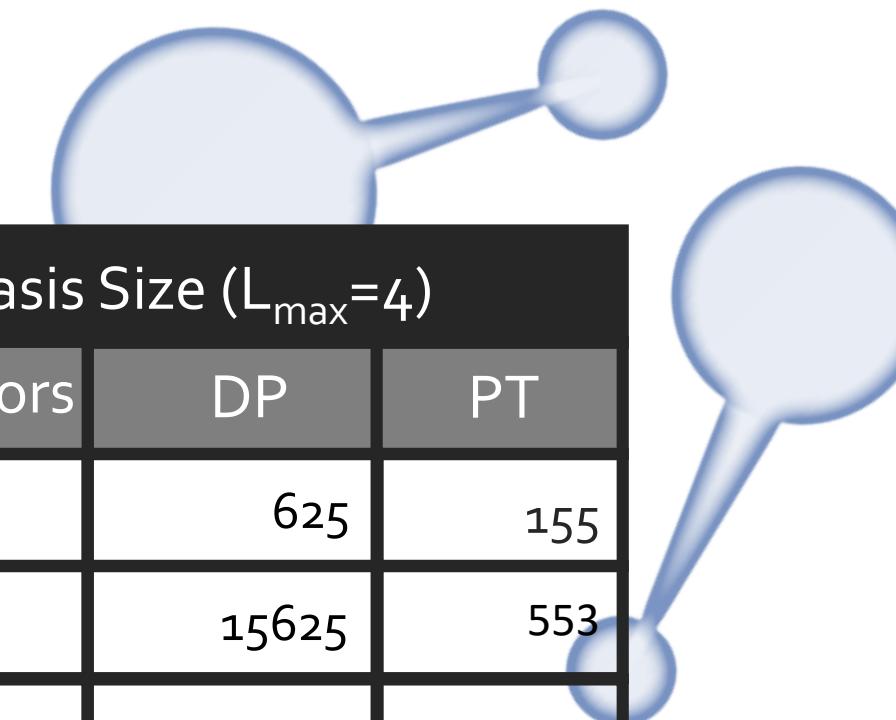


Polyad Truncation

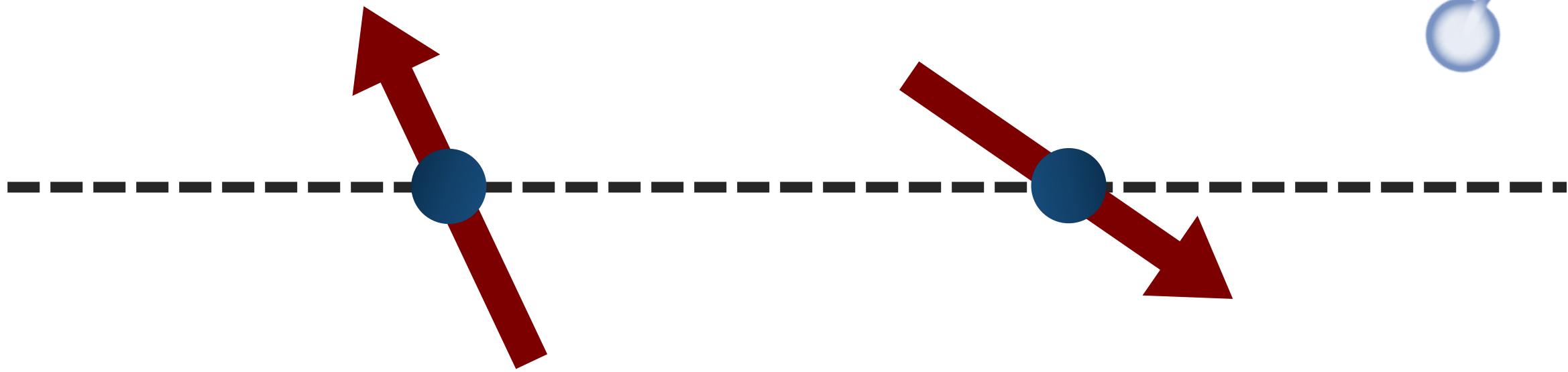
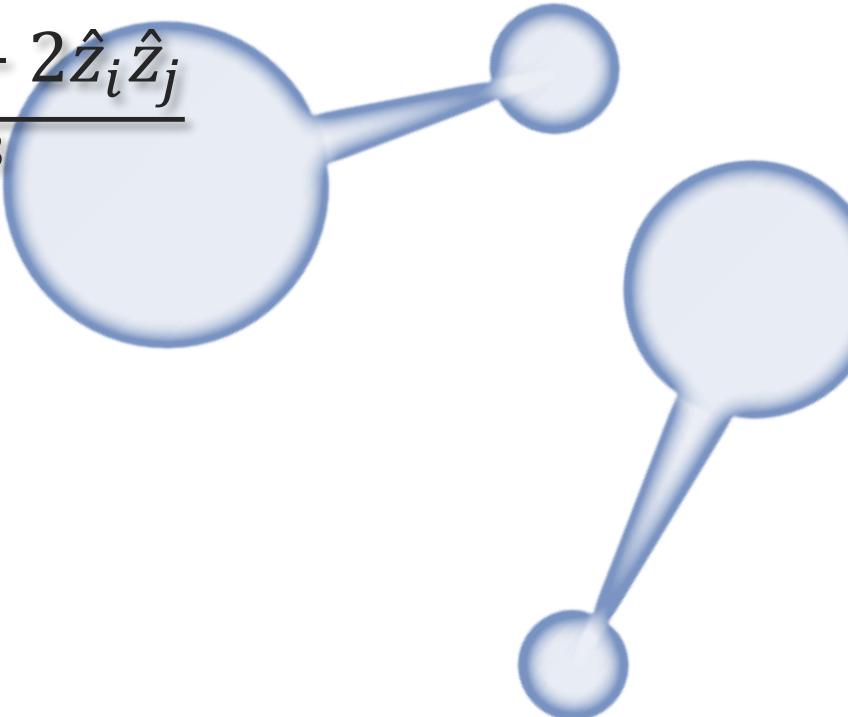




Basis Size ($L_{\max}=4$)		
#of Rotors	DP	PT
2	625	155
3	15625	553
4	390625	1462
5	9765625	3206
6	244140625	6190



$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j - i)^3}$$



Conclusions

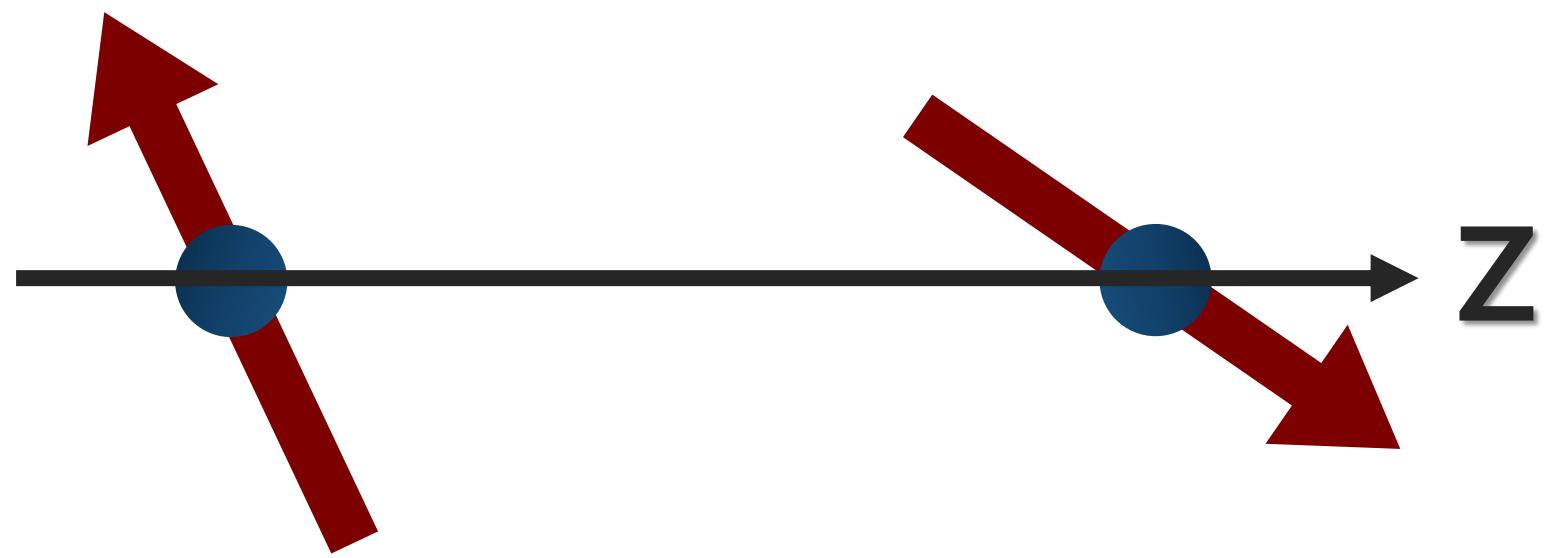
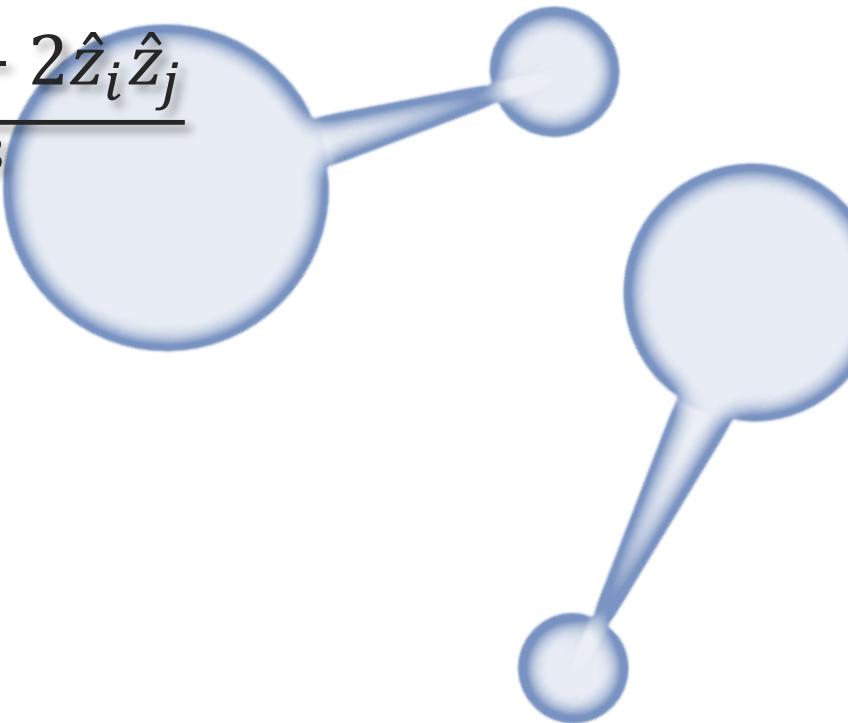
Confined Water

Dipole Chains

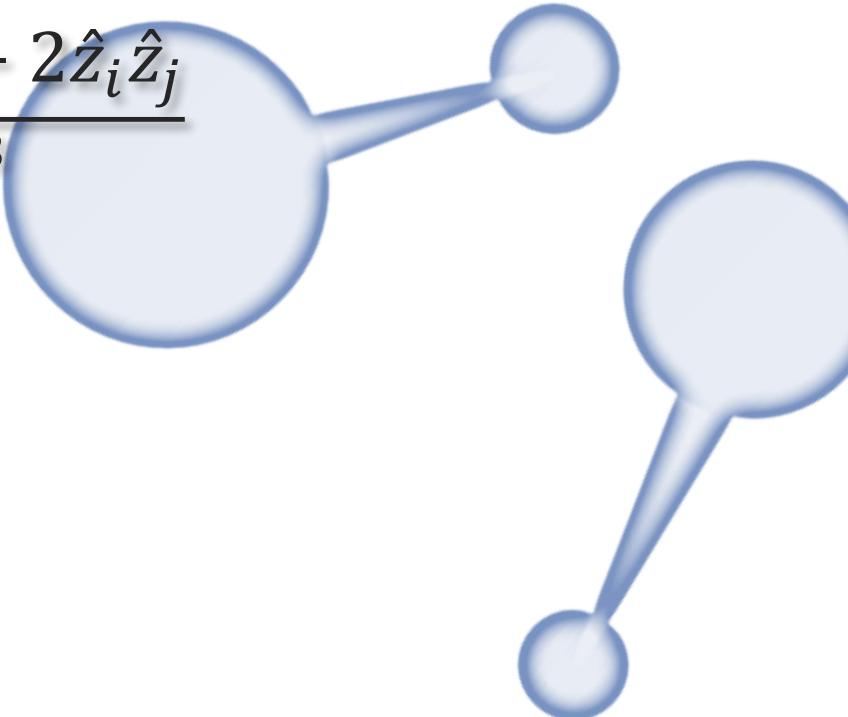
Hydrogen Clusters

Overview

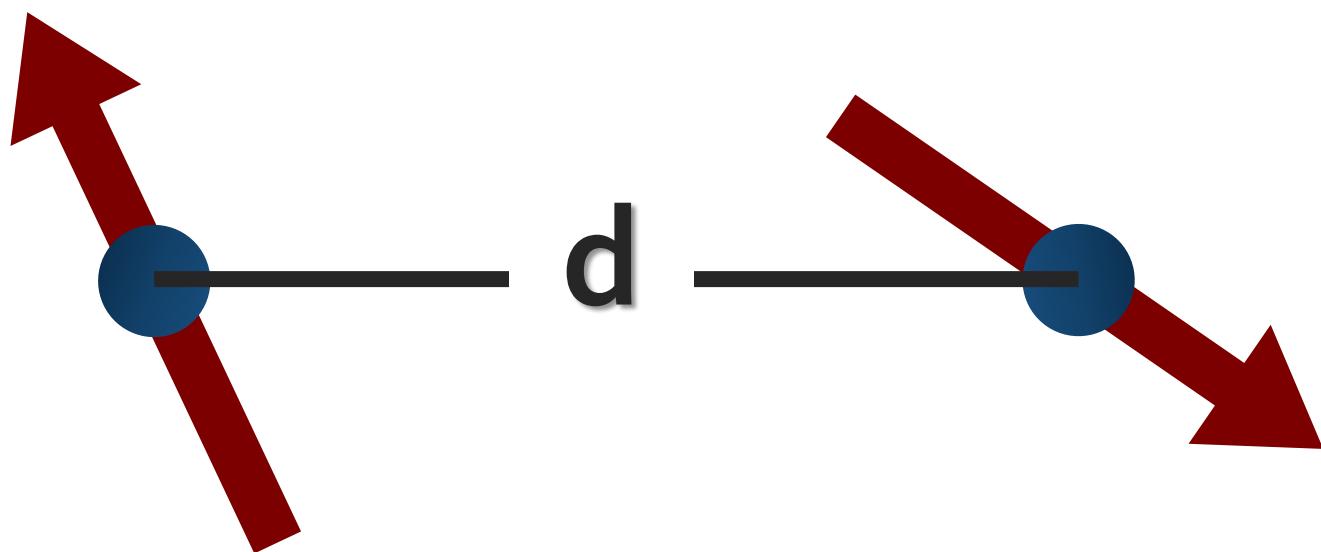
$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j - i)^3}$$



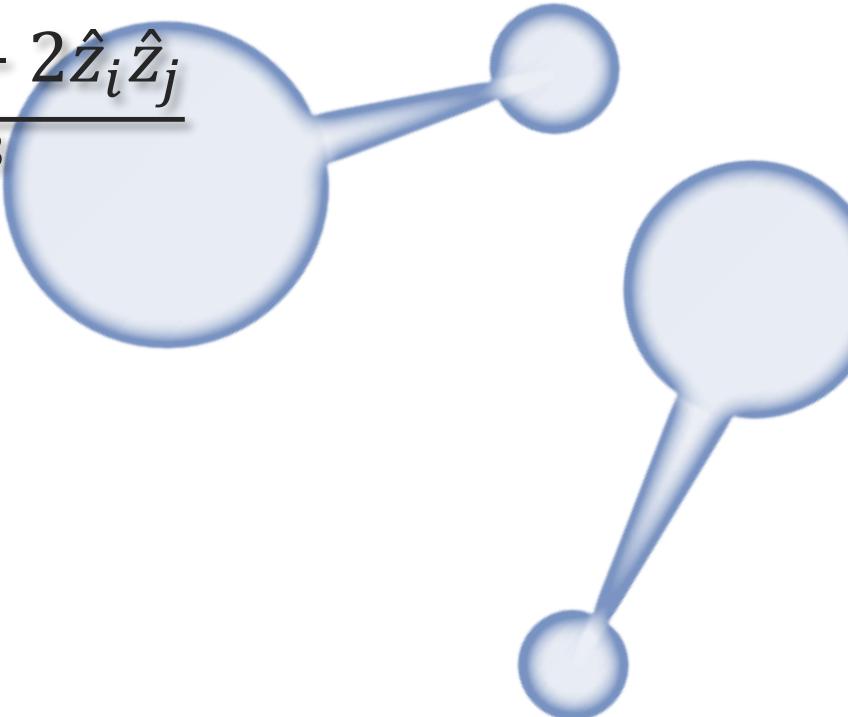
$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j - i)^3}$$



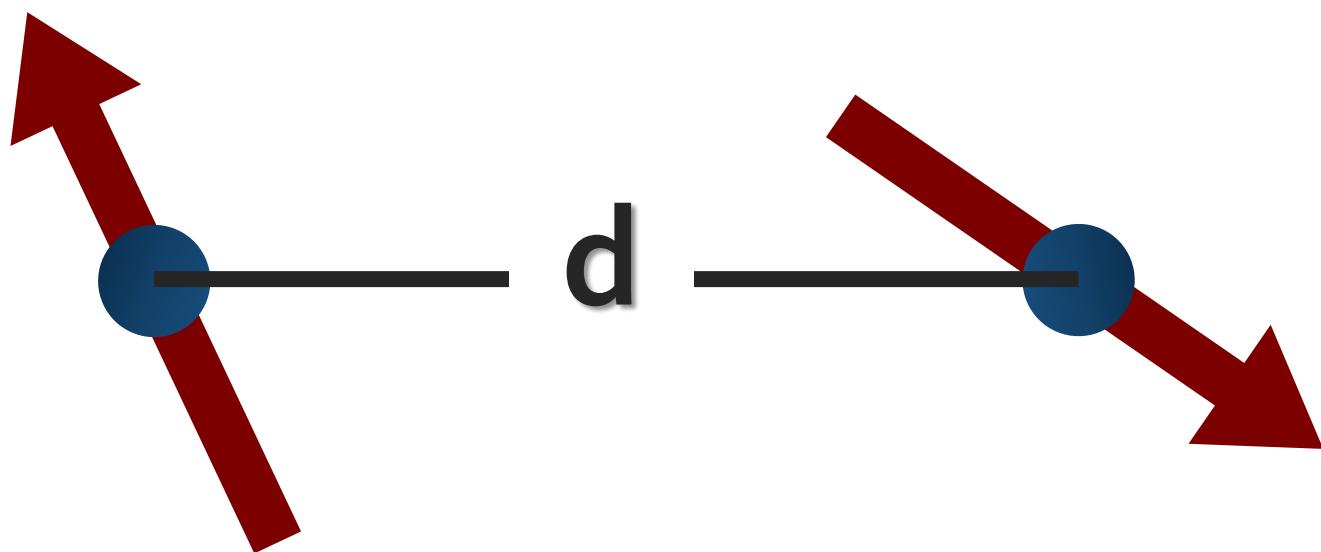
Lattice Spacing



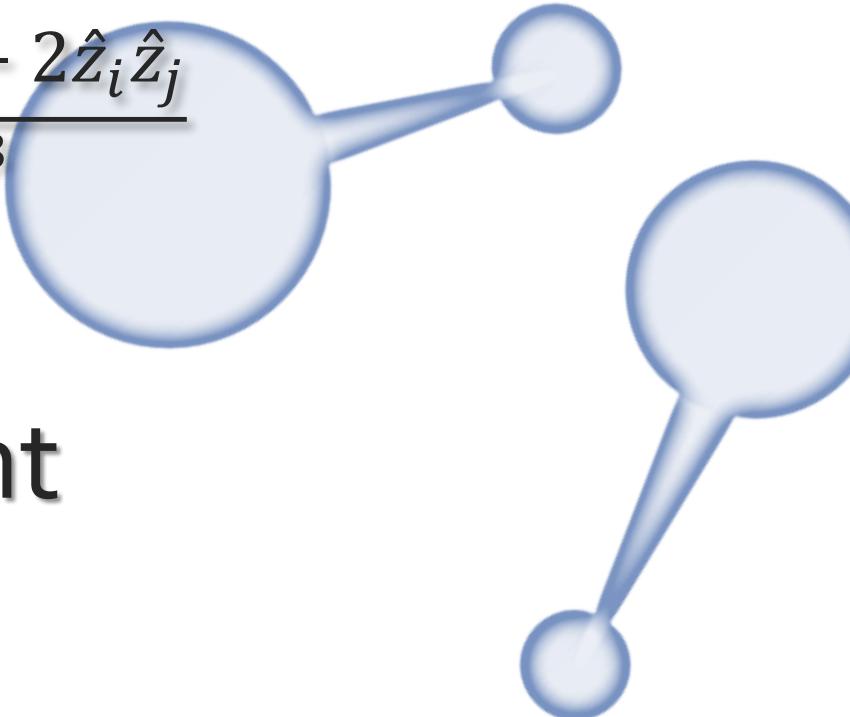
$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j - i)^3}$$



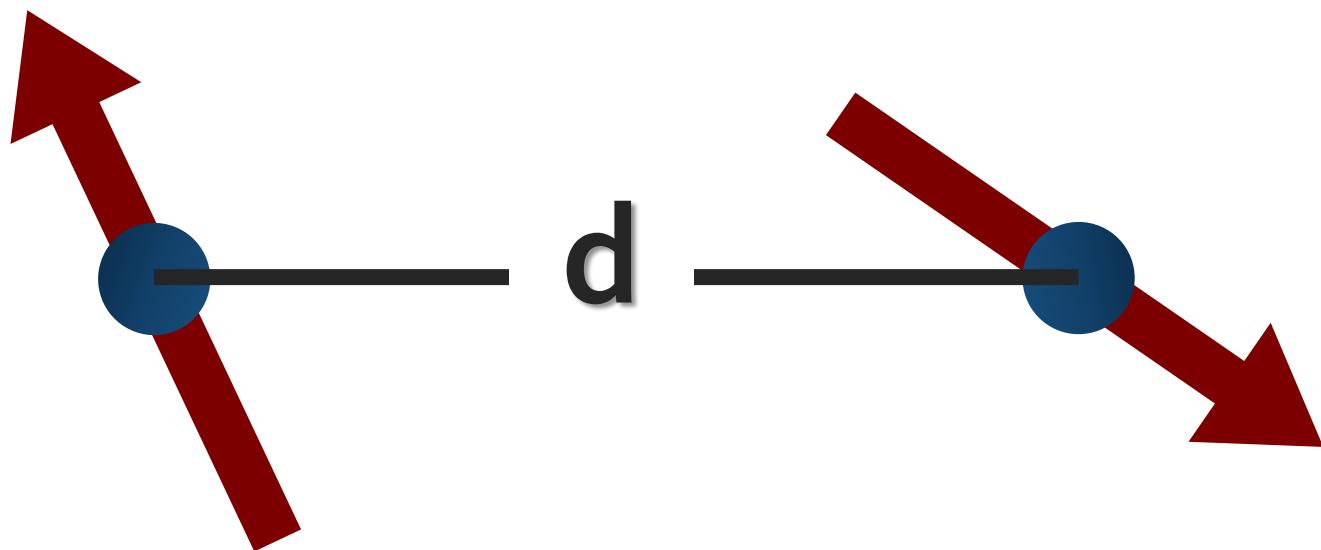
H-F: 10.05 Å



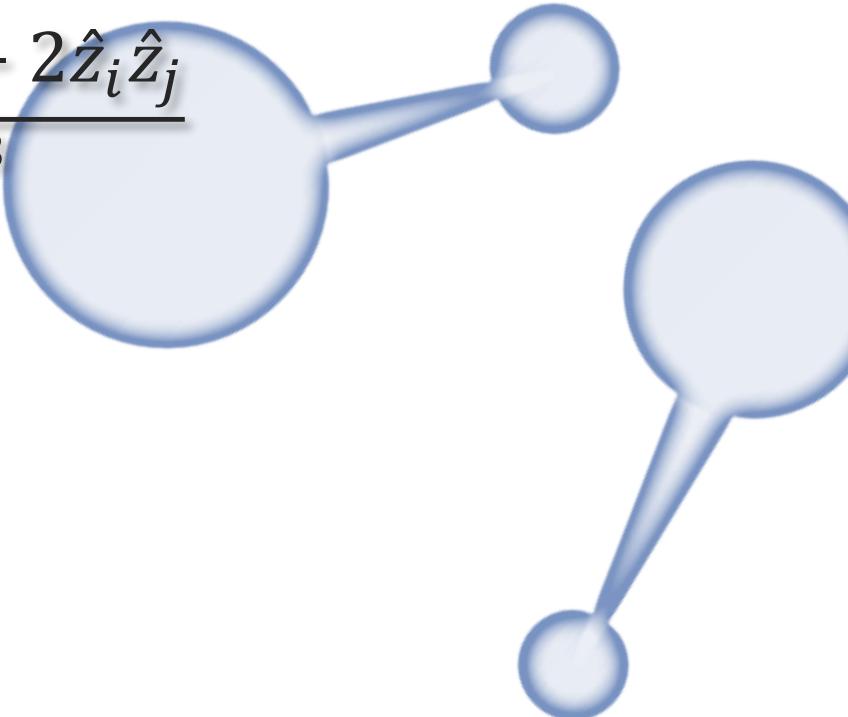
$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j - i)^3}$$



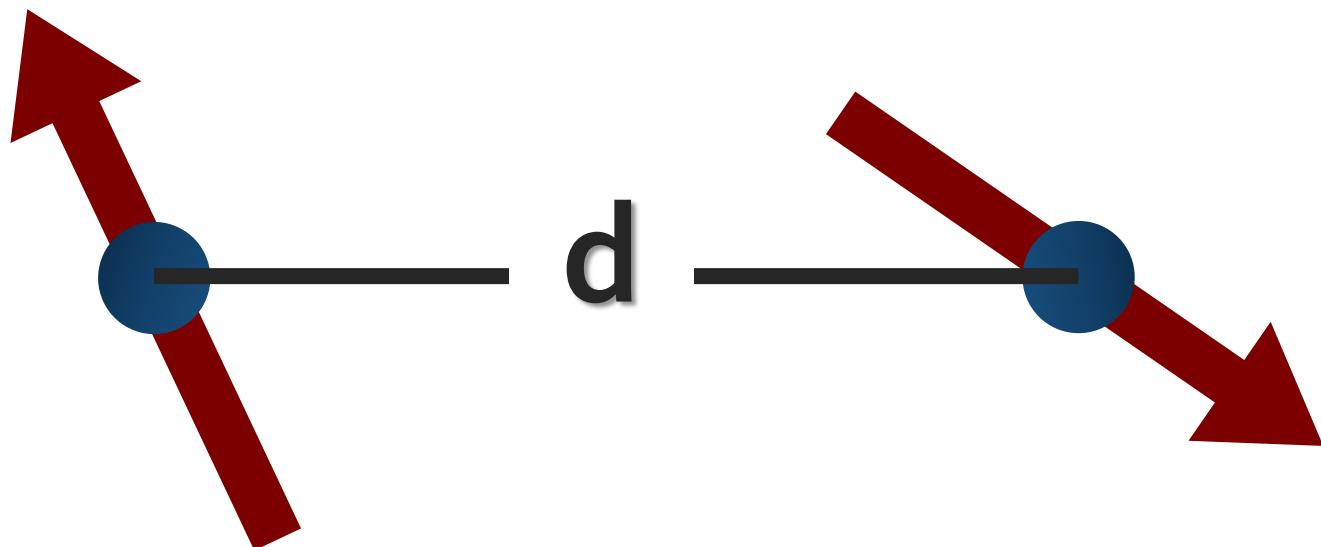
Rotational constant



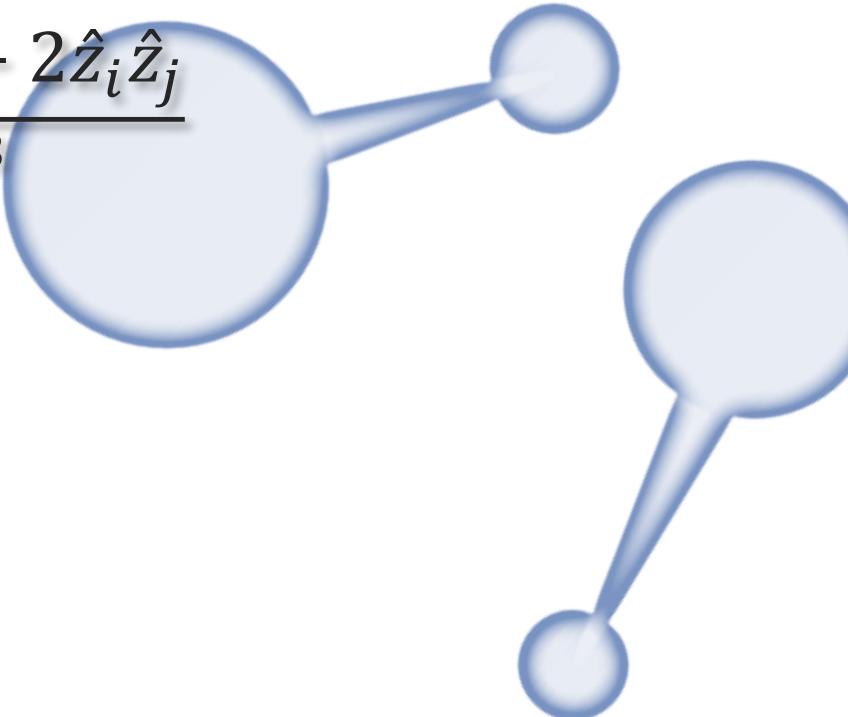
$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j-i)^3}$$



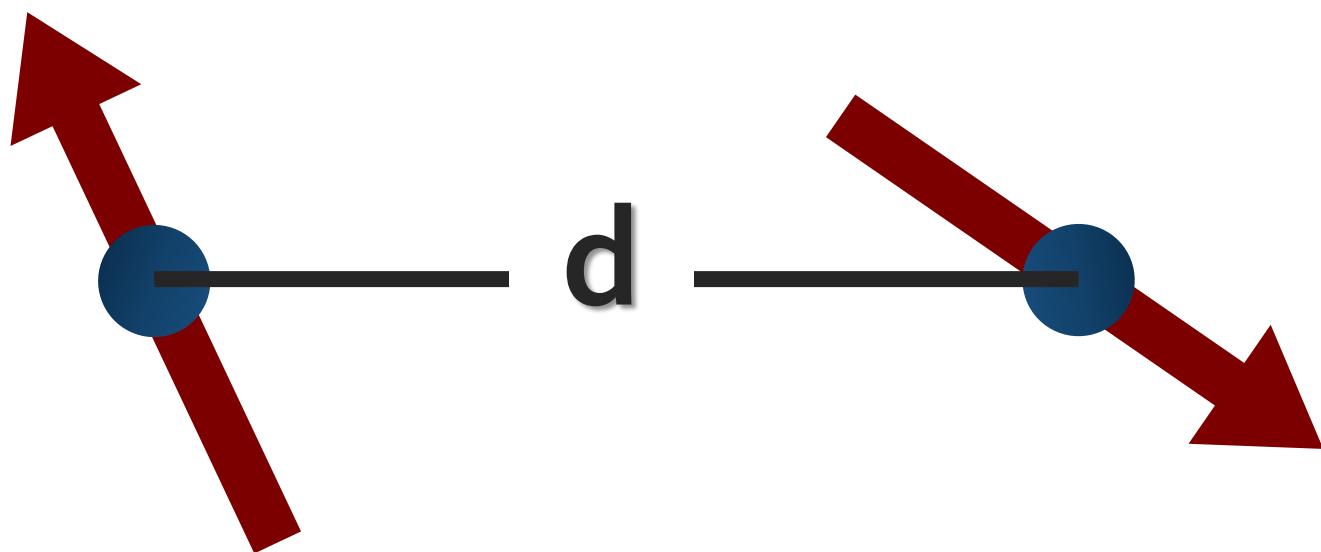
H-F: 20.96 cm⁻¹



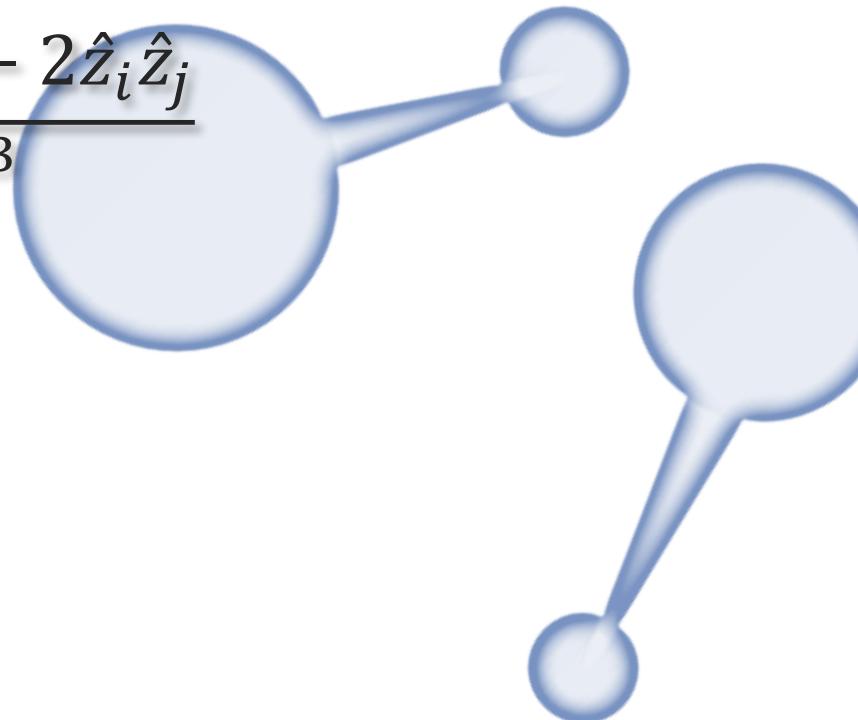
$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j - i)^3}$$



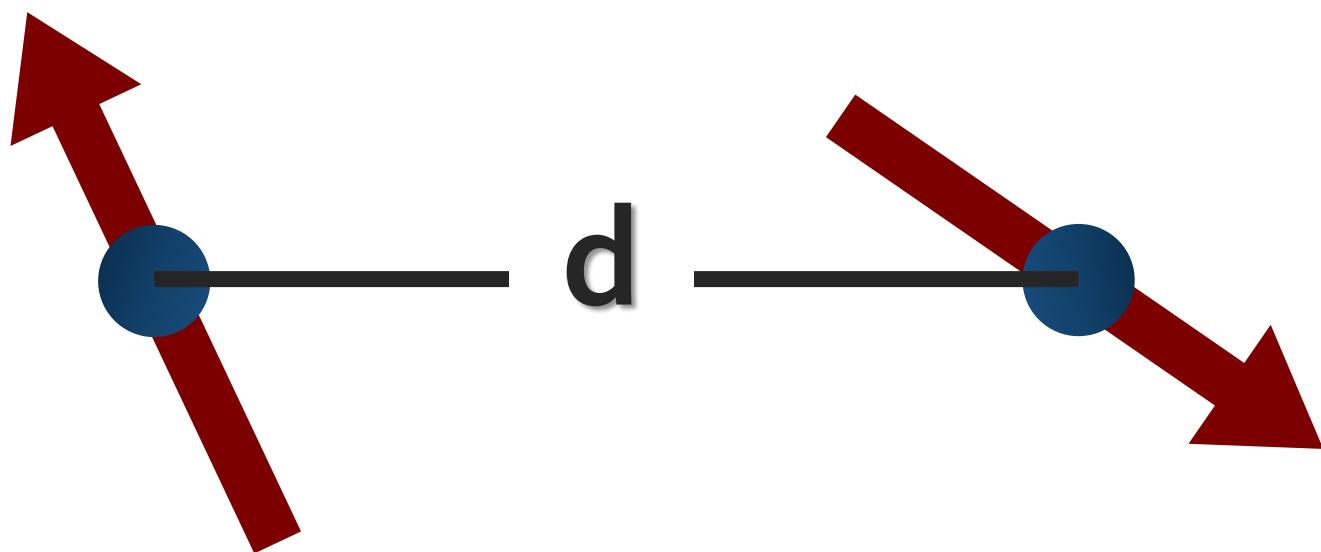
Dipole Moment



$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j - i)^3}$$

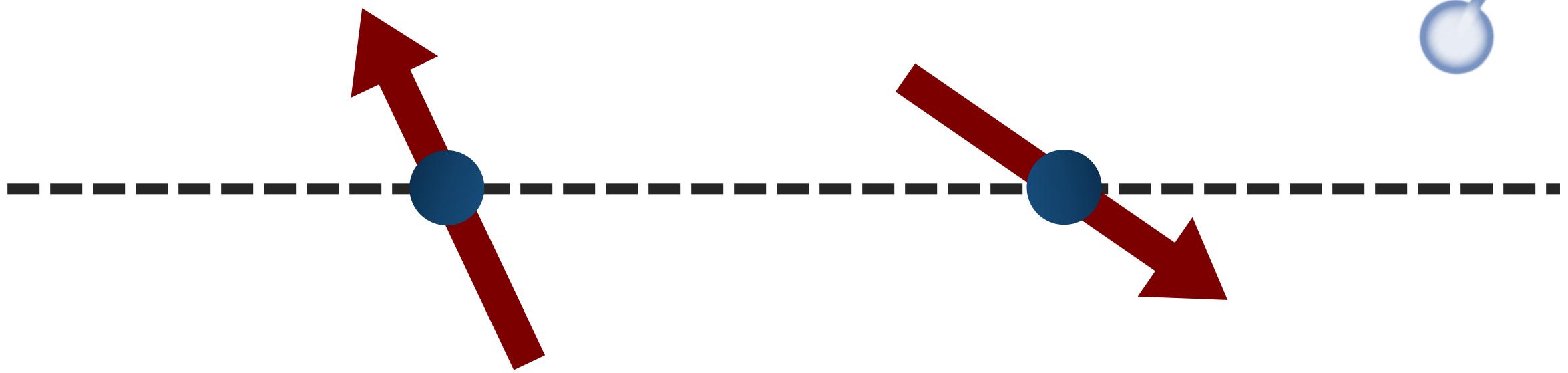


H-F: 1.86 debye

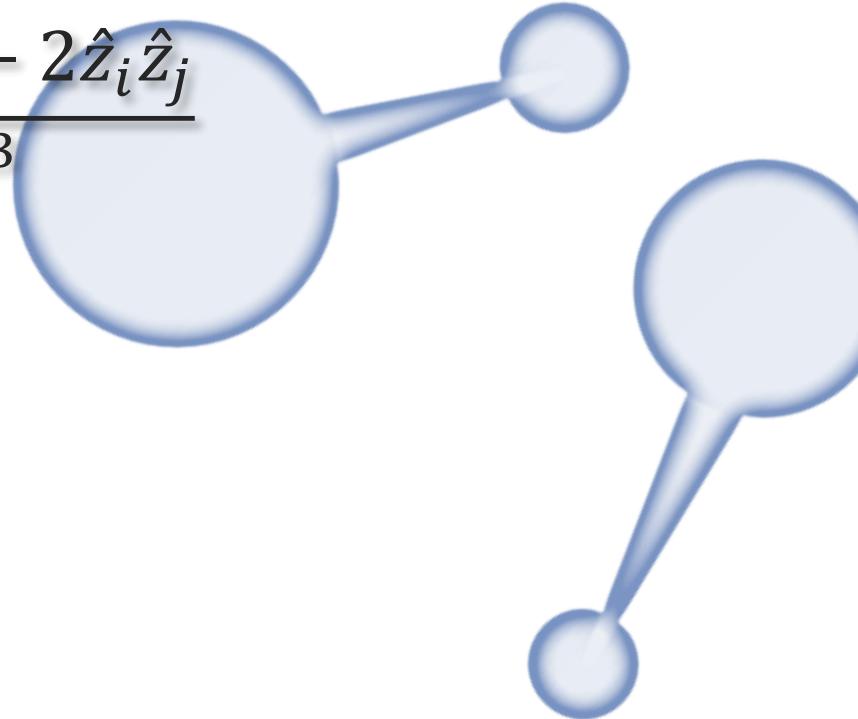


$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j - i)^3}$$

Natural Length Scale

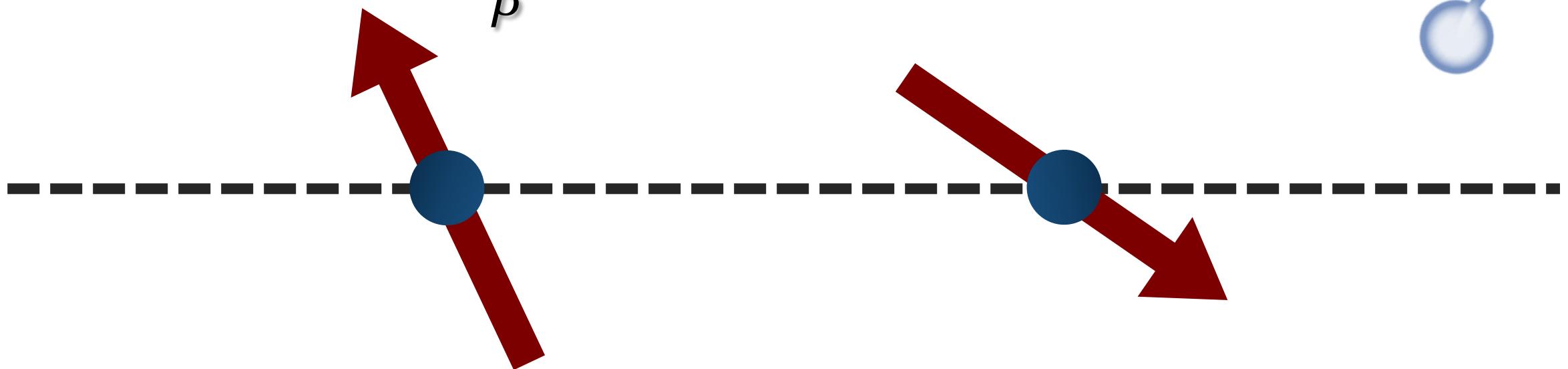


$$H = \alpha \sum_{i=1}^N \hat{l}_i^2 + \frac{\beta}{d^3} \sum_{i < j} \frac{\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j - 2 \hat{z}_i \hat{z}_j}{(j-i)^3}$$



Natural Length Scale

$$\frac{\alpha}{\beta} \approx \delta^3 \quad \delta \approx 9.4 \approx d$$



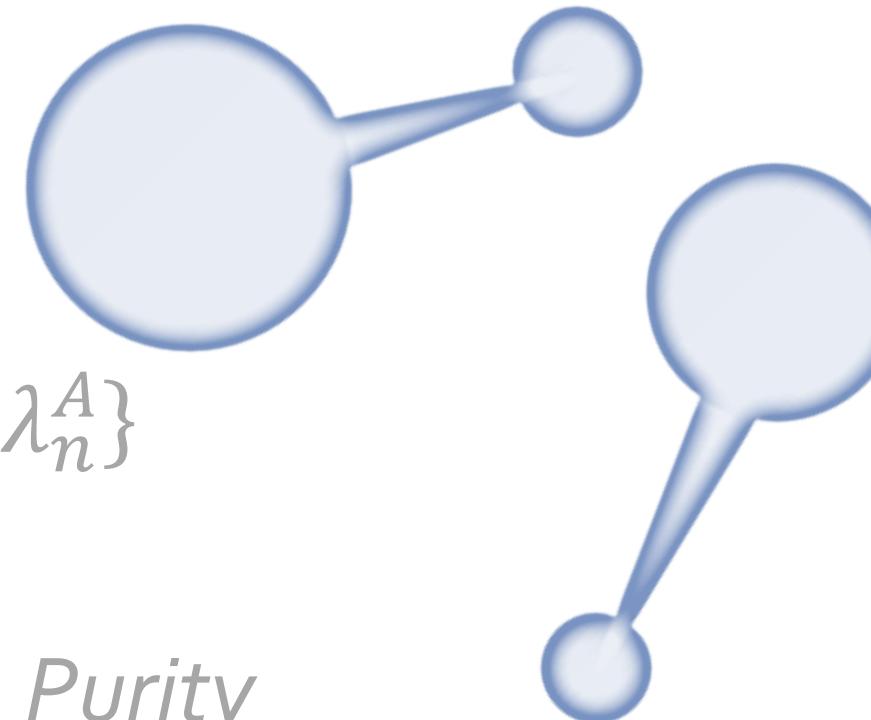


Reduced Density Matrix

$$\rho = |\psi_0\rangle \langle \psi_0|$$

$$\rho_A = \text{Tr}_B \rho$$

$$\langle \phi' | \rho_A | \phi \rangle \Rightarrow \{\lambda_0^A, \lambda_1^A, \dots \lambda_n^A\}$$



von Neumann Entropy

$$S = - \sum_{i=0}^{N_A} \lambda_i^A \ln \lambda_i^A$$

Purity

$$P = \sum_{i=0}^{N_A} (\lambda_i^A)^2$$

$$\rho = |\psi_0\rangle \langle \psi_0|$$

$$\rho_A = \text{Tr}_B \rho$$

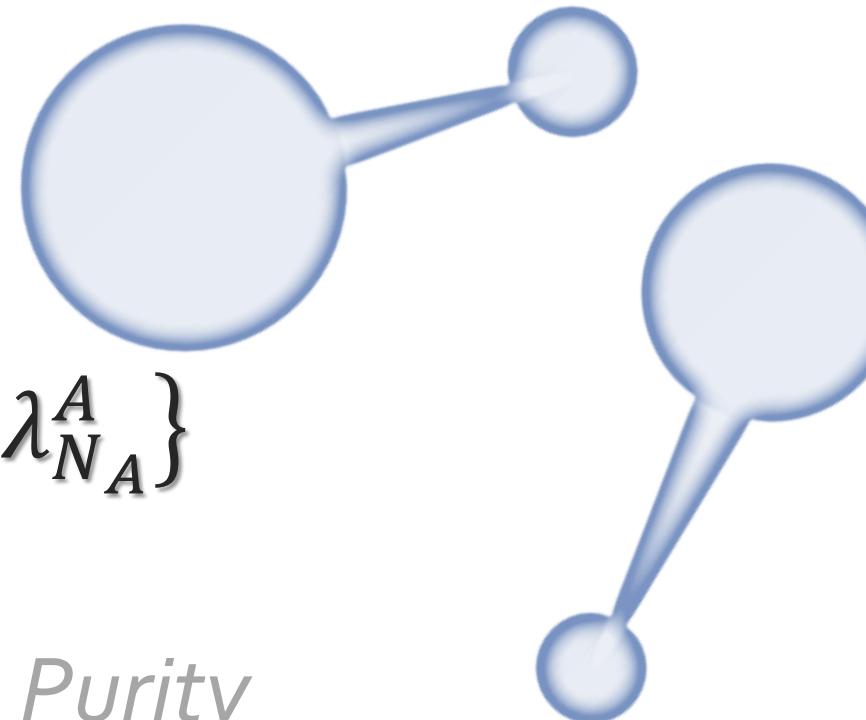
$$\langle \phi' | \rho_A | \phi \rangle \Rightarrow \{\lambda_0^A, \lambda_1^A, \dots \lambda_{N_A}^A\}$$

von Neumann Entropy

$$S = - \sum_{i=0}^{N_A} \lambda_i^A \ln \lambda_i^A$$

Purity

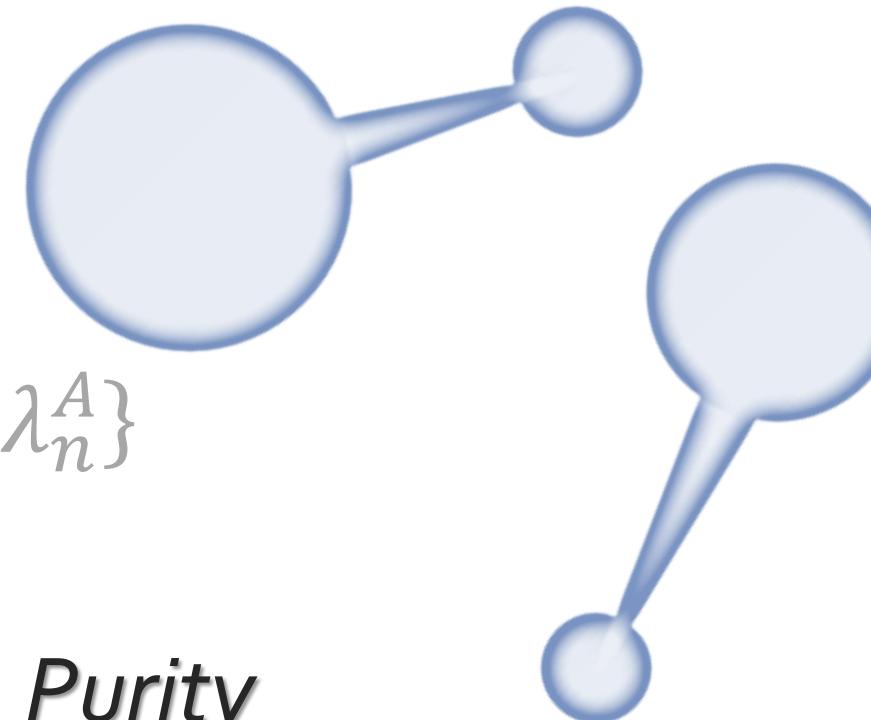
$$P = \sum_{i=0}^{N_A} (\lambda_i^A)^2$$



$$\rho = |\psi_0\rangle \langle \psi_0|$$

$$\rho_A = \text{Tr}_B \rho$$

$$\langle \phi' | \rho_A | \phi \rangle \Rightarrow \{\lambda_0^A, \lambda_1^A, \dots \lambda_n^A\}$$

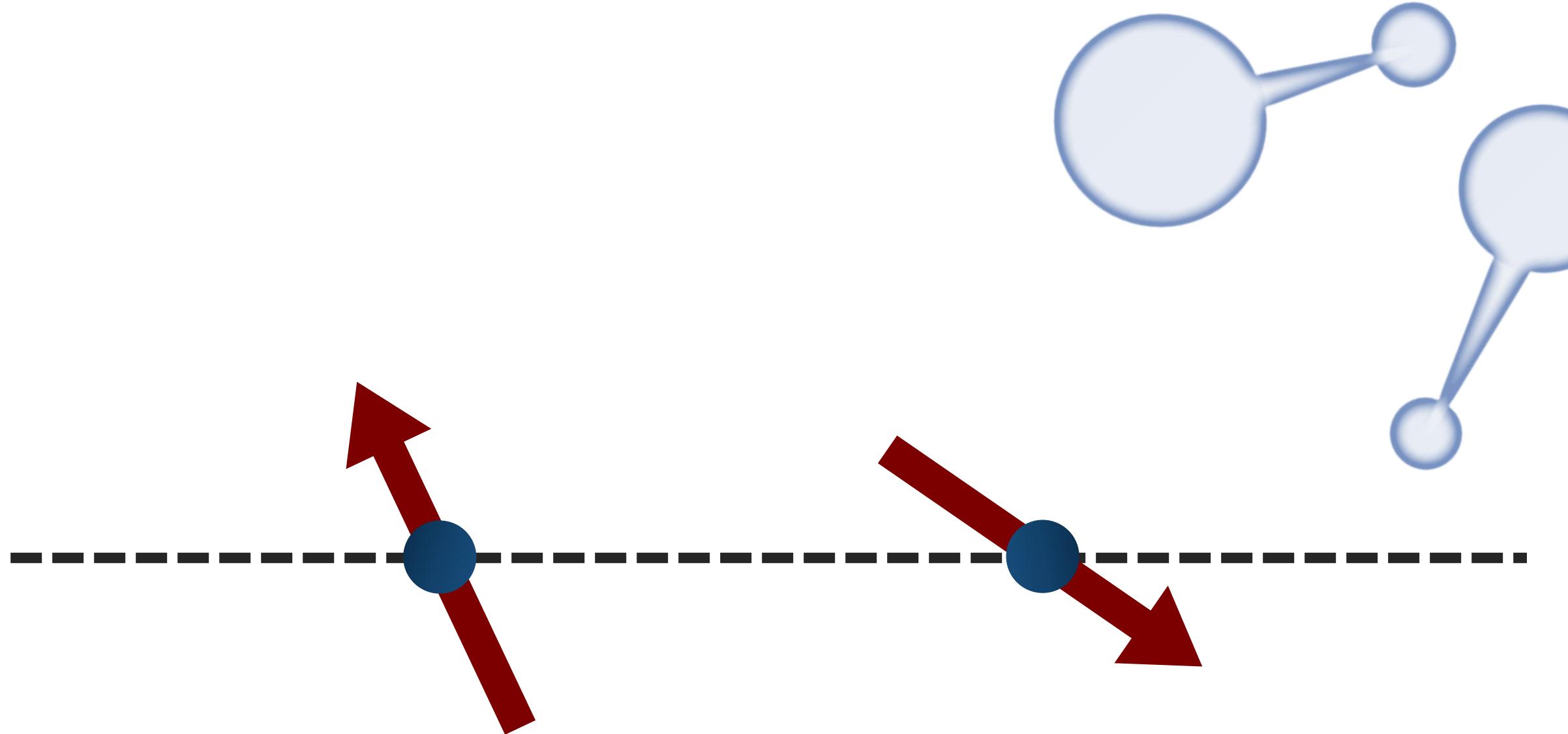


von Neumann Entropy

$$S = - \sum_{i=0}^{N_A} \lambda_i^A \ln \lambda_i^A$$

Purity

$$P = \sum_{i=0}^{N_A} (\lambda_i^A)^2$$



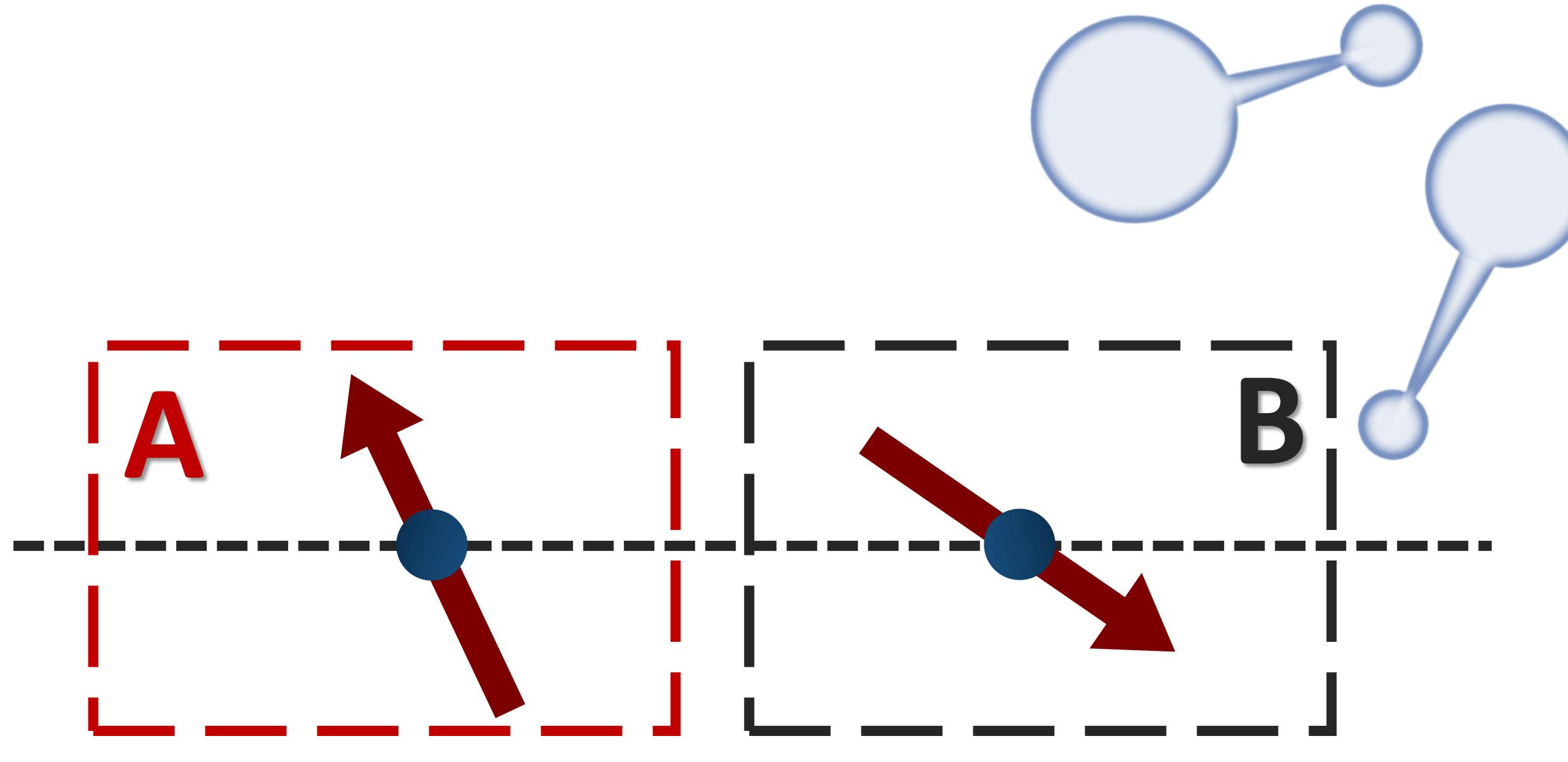
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Dipole Chains

Hydrogen Clusters

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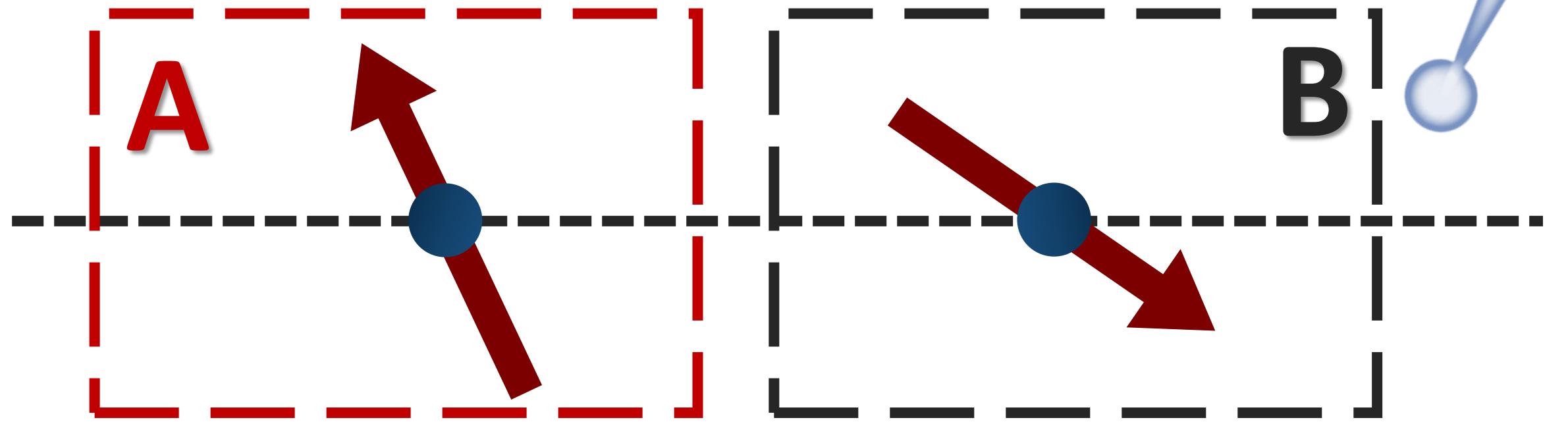
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$$|I\rangle = |l_1 m_1 l_2 m_2\rangle = |l_1 m_1\rangle \otimes |l_2 m_2\rangle$$



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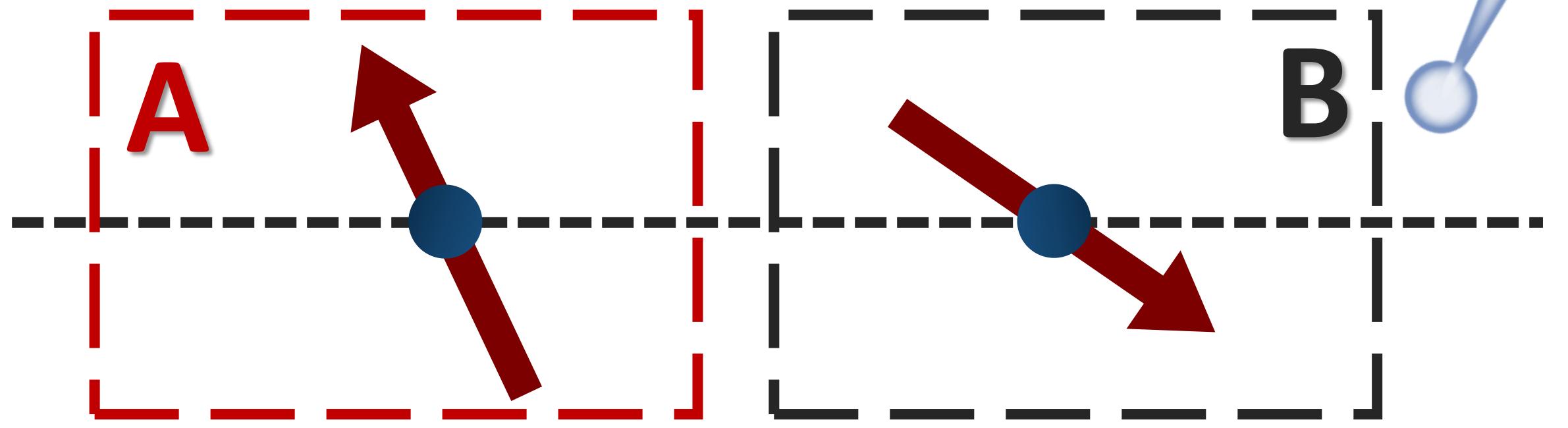
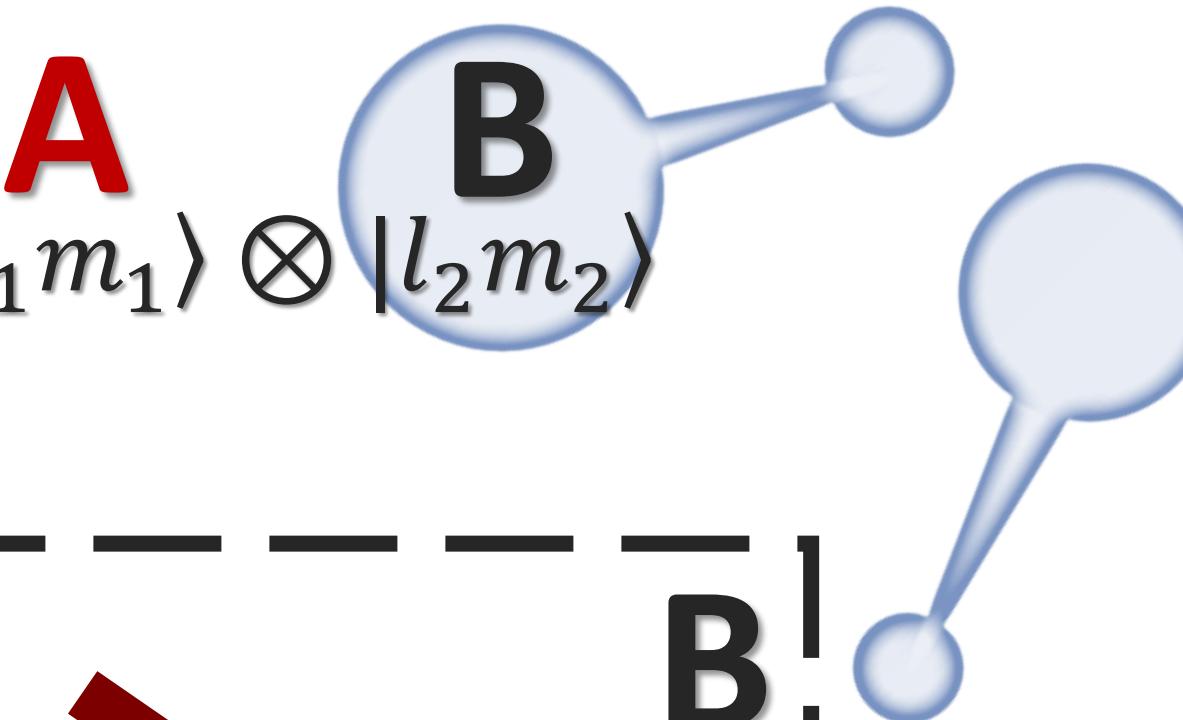
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$$|I\rangle = |l_1 m_1 l_2 m_2\rangle = |l_1 m_1\rangle \otimes |l_2 m_2\rangle$$



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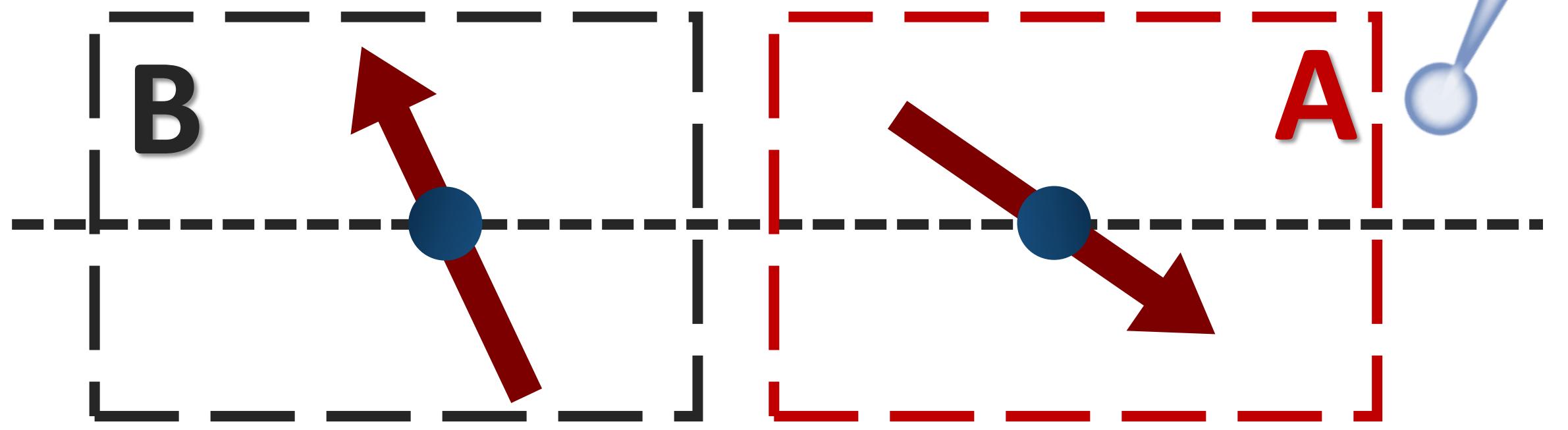
Hydrogen Clusters

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$$|I\rangle = |l_1 m_1 l_2 m_2\rangle = |l_1 m_1\rangle \otimes |l_2 m_2\rangle$$

B

A



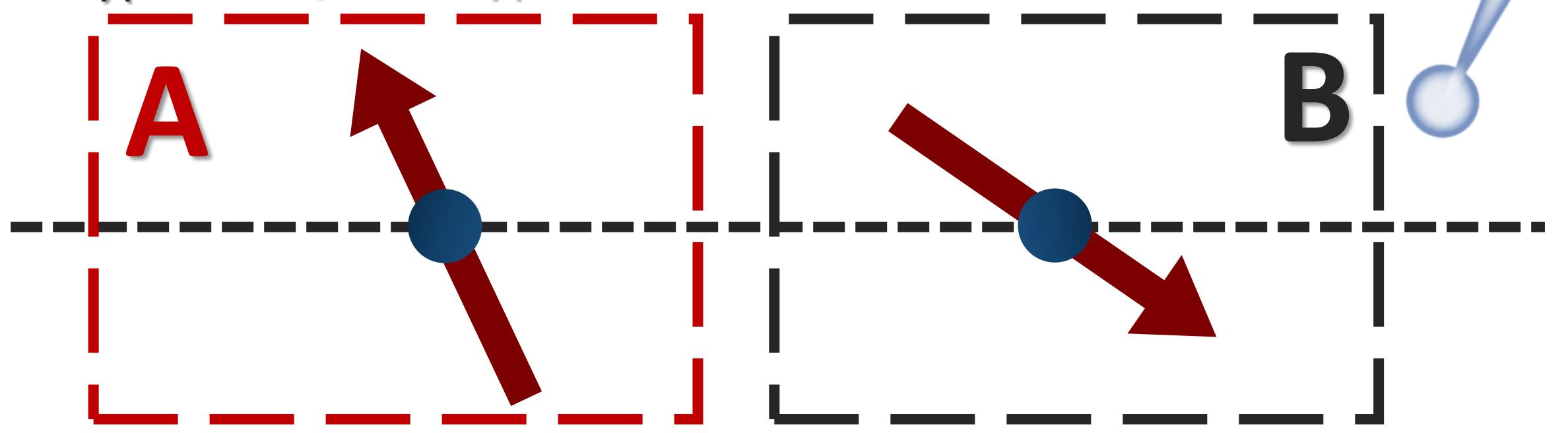
$$|I\rangle = |l_1 m_1 l_2 m_2\rangle = |l_1 m_1\rangle \otimes |l_2 m_2\rangle$$

A

B

$$S_A = 0.146$$

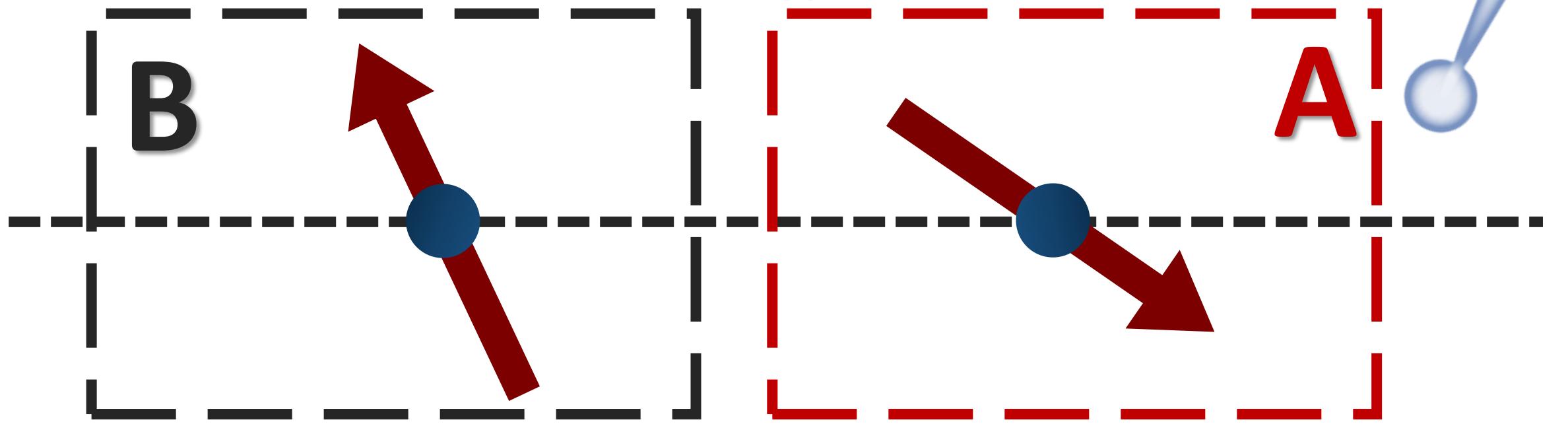
$$P_A = 0.947$$



$$|I\rangle = |l_1 m_1 l_2 m_2\rangle = |l_1 m_1\rangle \otimes |l_2 m_2\rangle$$

B
A

$$S_A = 0.146 \quad P_A = 0.947$$



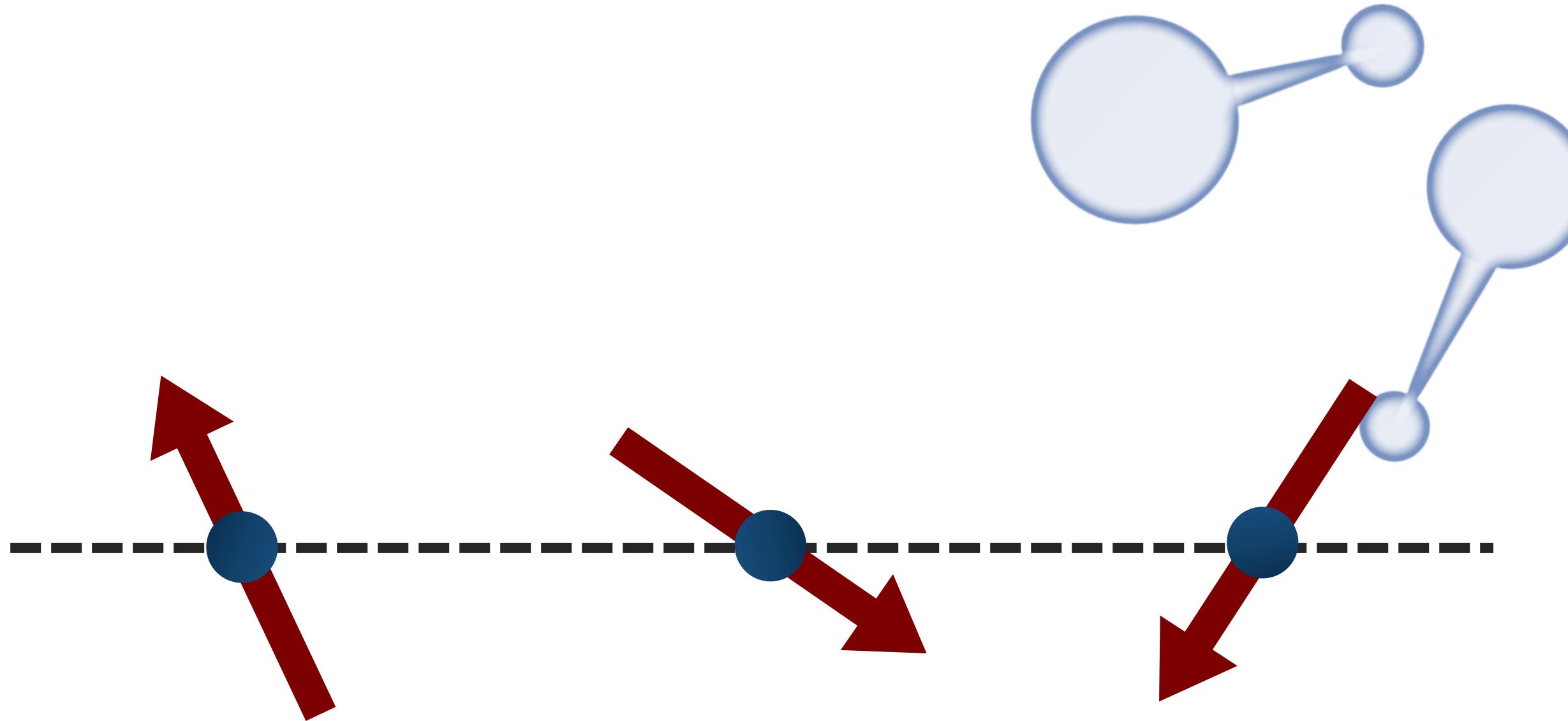
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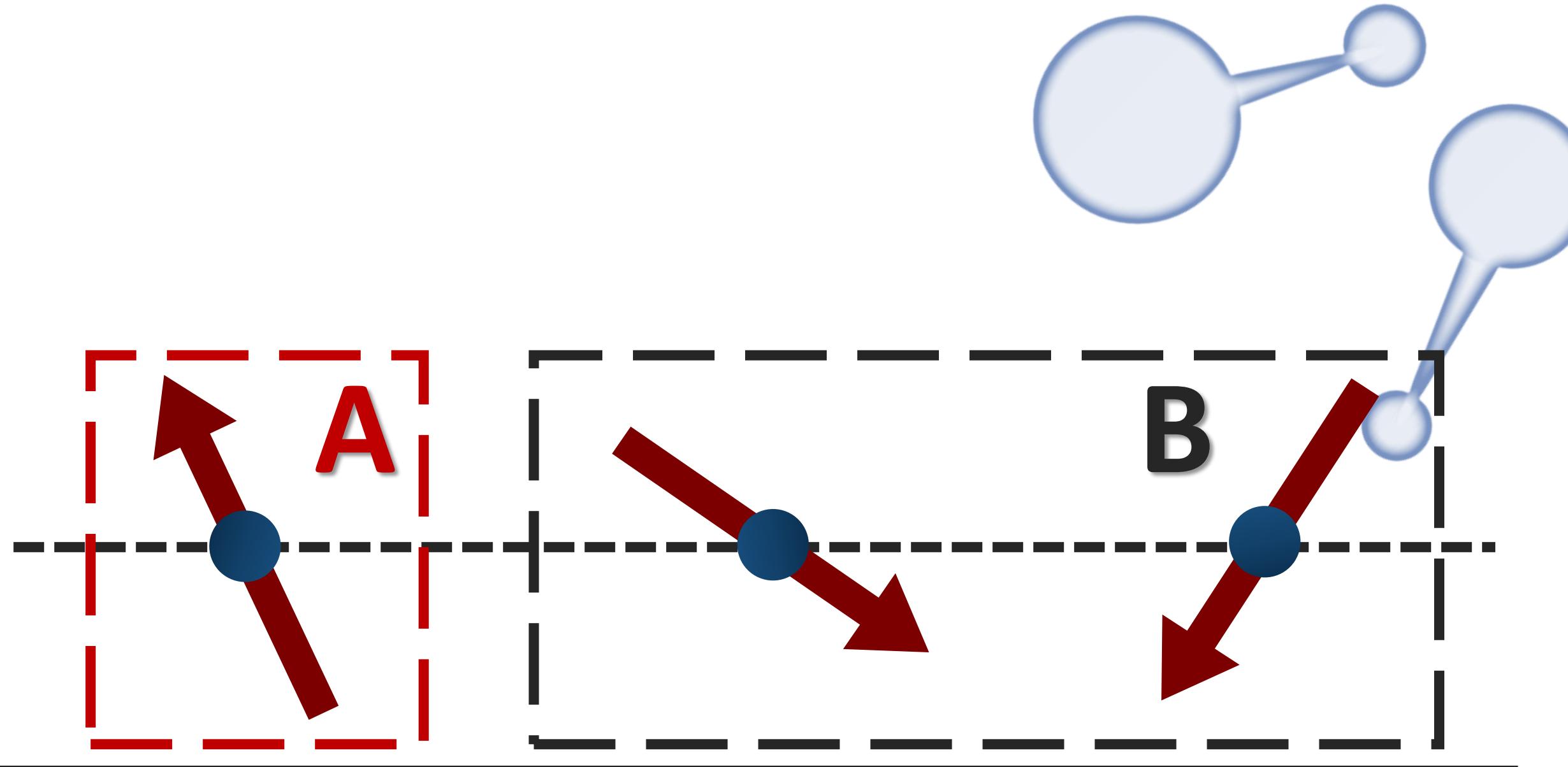
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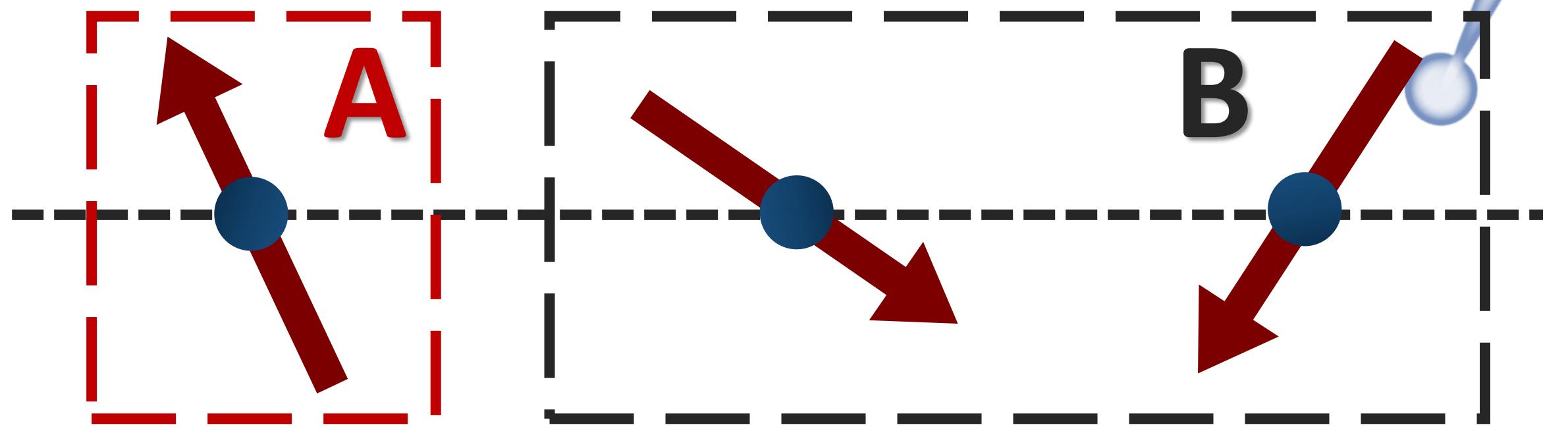
Hydrogen Clusters

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$$|I\rangle = |l_1 m_1 l_2 m_2 l_3 m_3\rangle = |l_1 m_1\rangle \otimes |l_2 m_2 l_3 m_3\rangle$$

A

B



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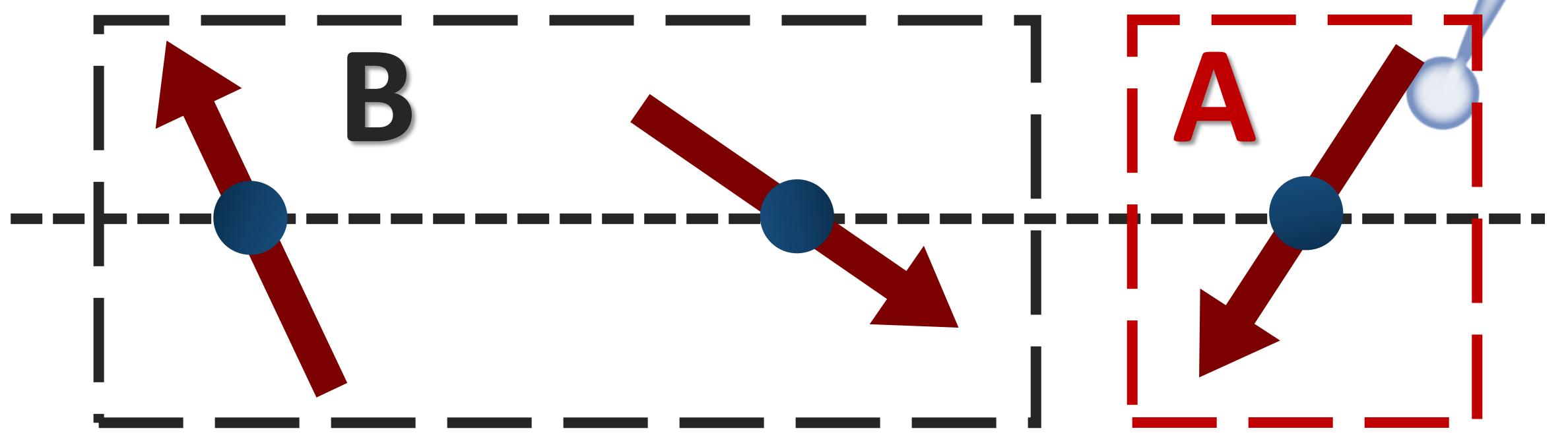
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Overview

$$|I\rangle = |l_1 m_1 l_2 m_2 l_3 m_3\rangle = |l_3 m_3\rangle \otimes |l_1 m_1 l_2 m_2\rangle$$

A

B



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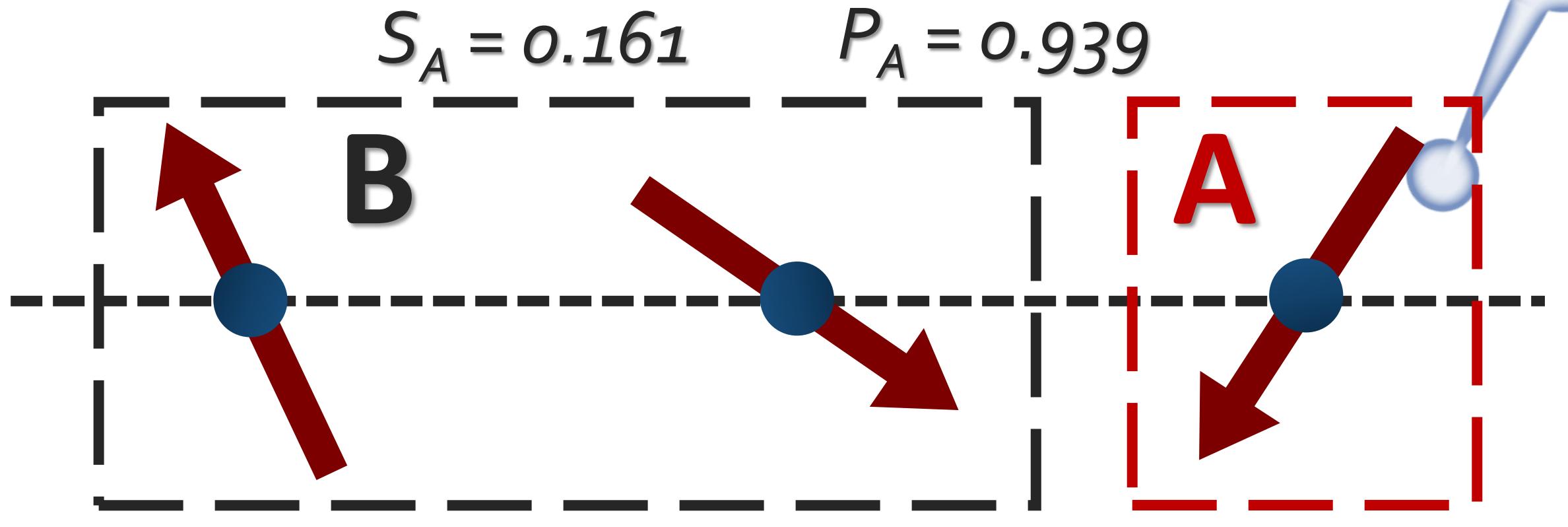
Hydrogen Clusters

Overview

$$|I\rangle = |l_1 m_1 l_2 m_2 l_3 m_3\rangle = |l_3 m_3\rangle \otimes |l_1 m_1 l_2 m_2\rangle$$

A

B



Conclusions

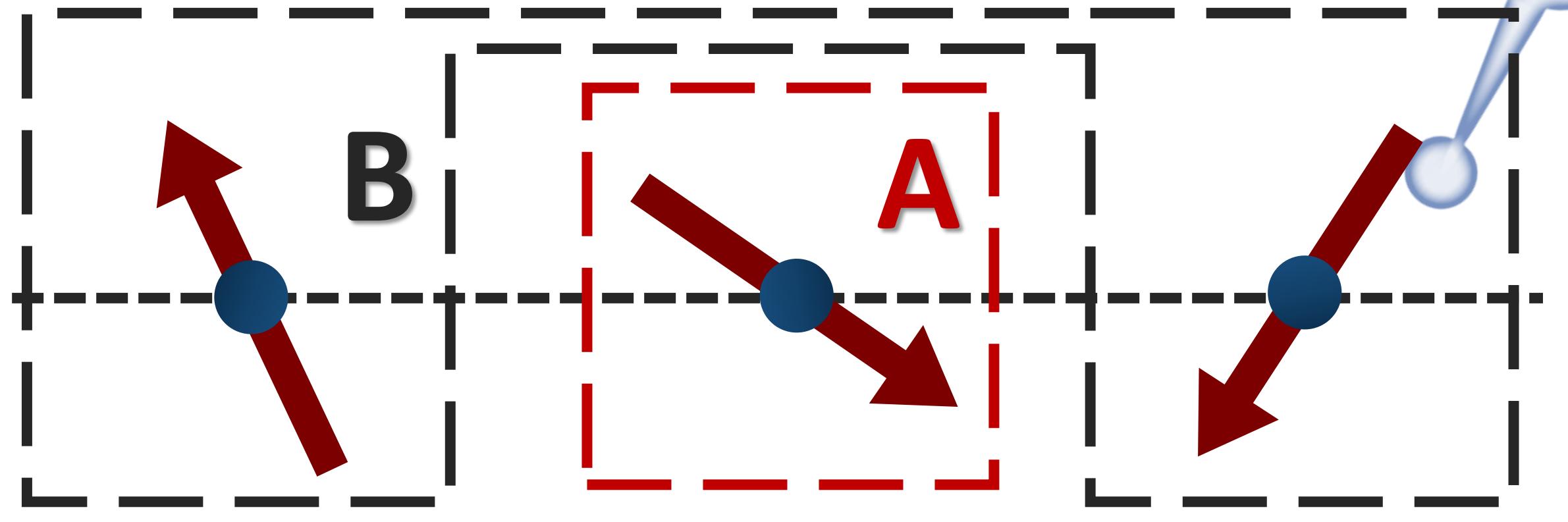
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$$|I\rangle = |l_1 m_1 l_2 m_2 l_3 m_3\rangle = |l_2 m_2\rangle \otimes |l_1 m_1 l_3 m_3\rangle$$



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$$\overline{S_A = 0.161}$$

$$\overline{S_A = 0.262}$$

$$\overline{S_A = 0.161}$$

Conclusions

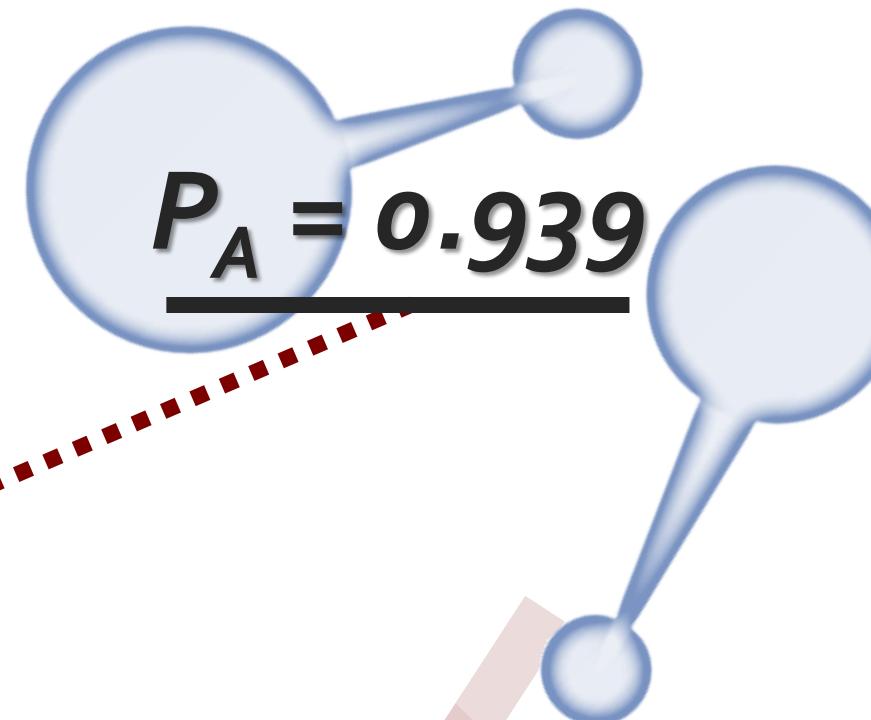
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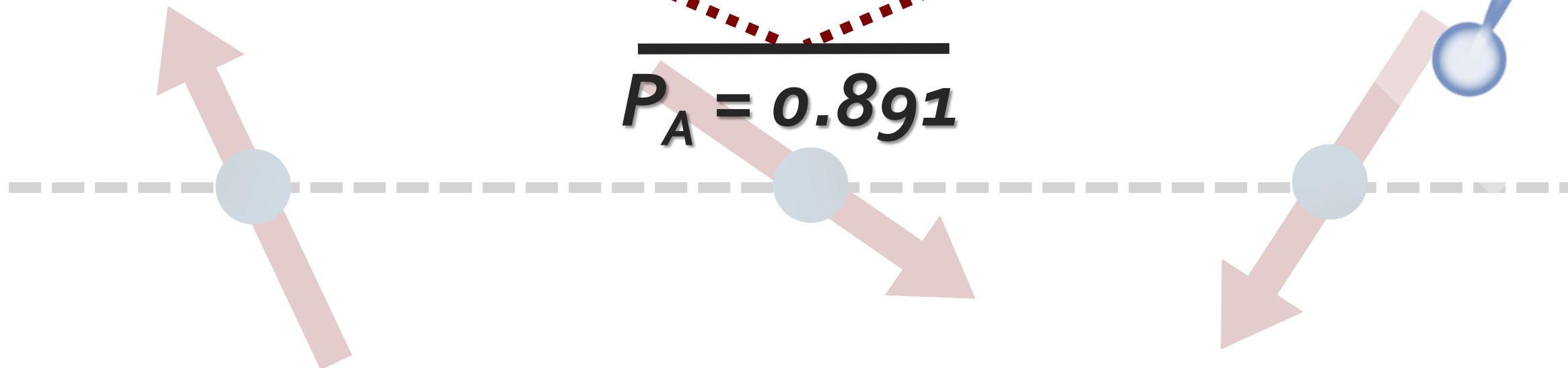
Hydrogen Clusters

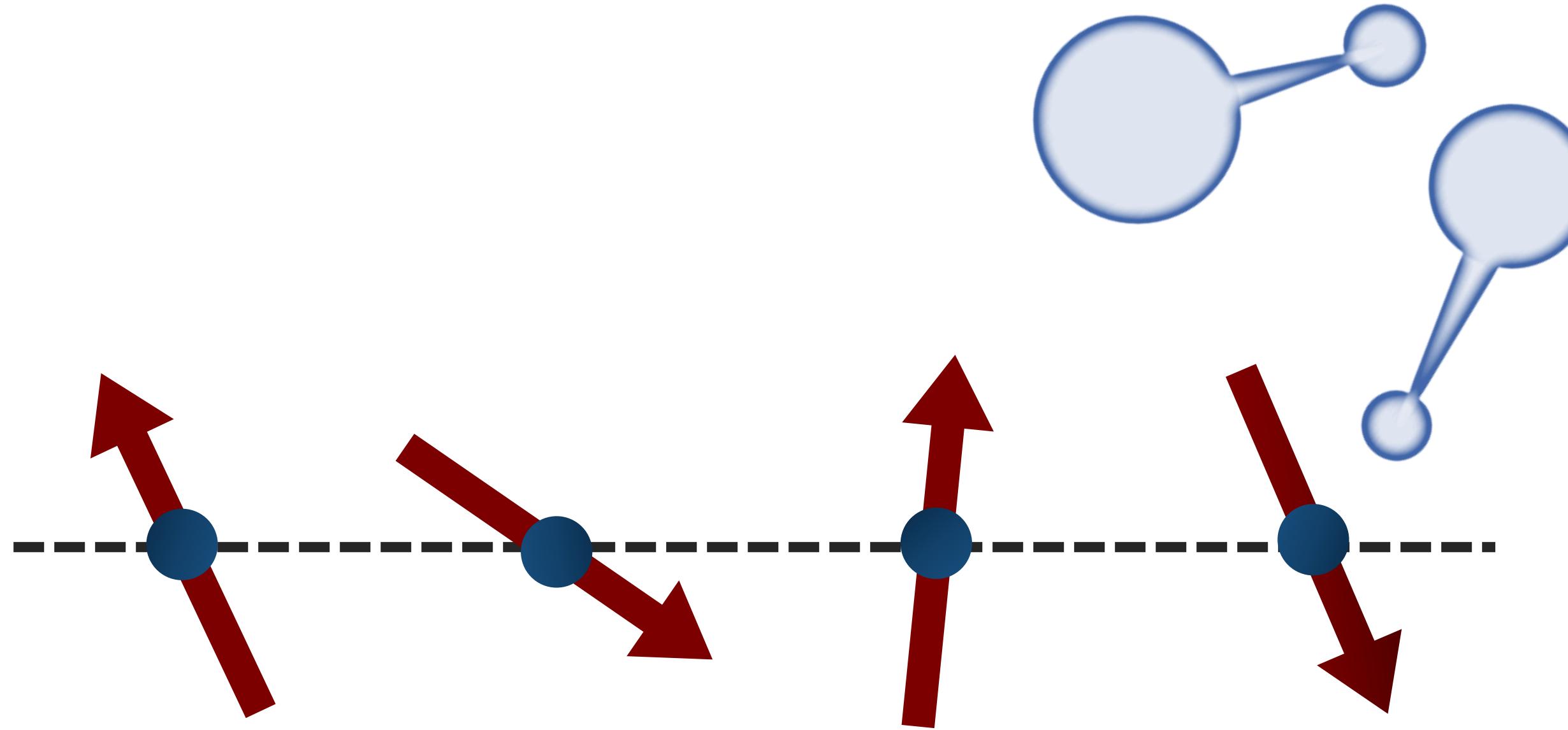
Overview

$P_A = 0.939$



$P_A = 0.891$





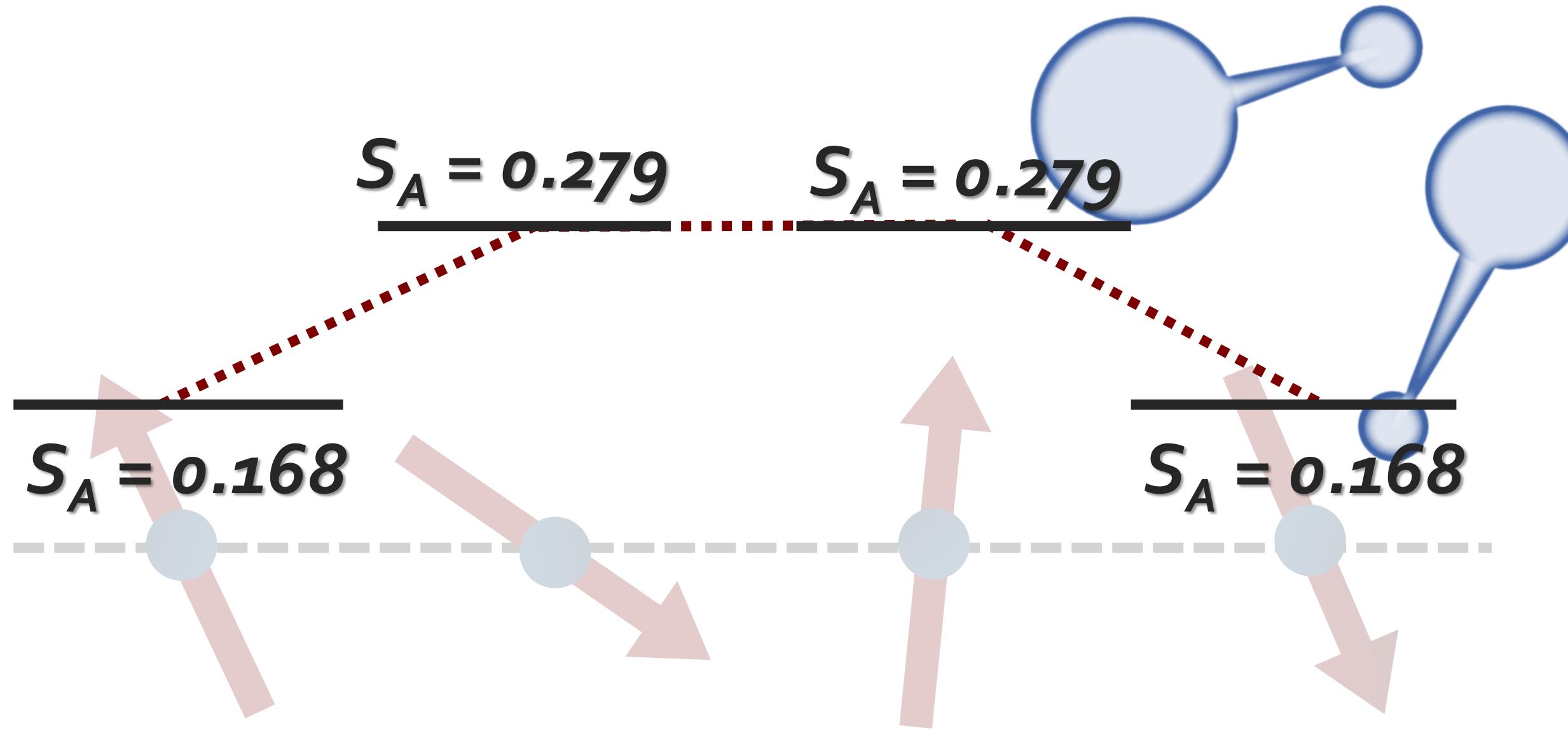
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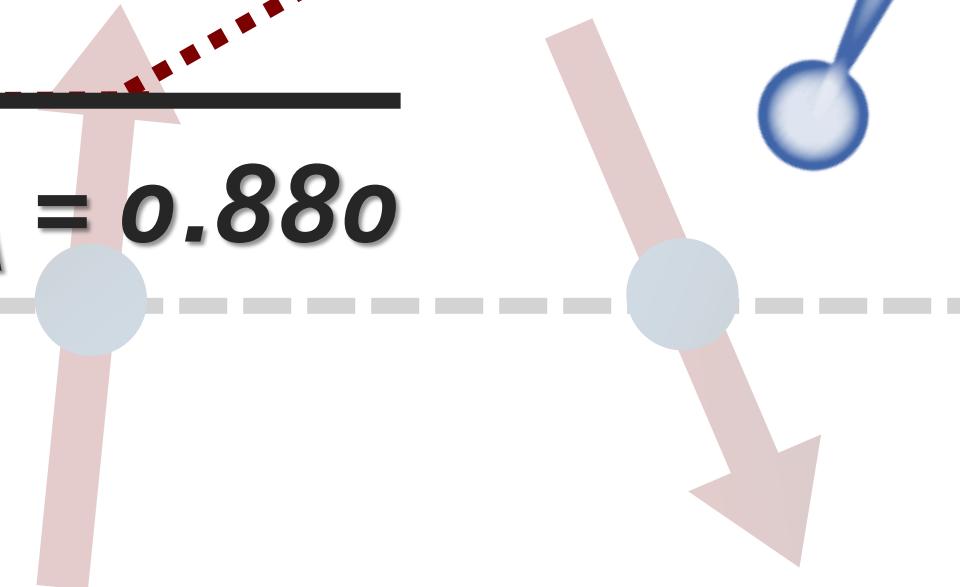
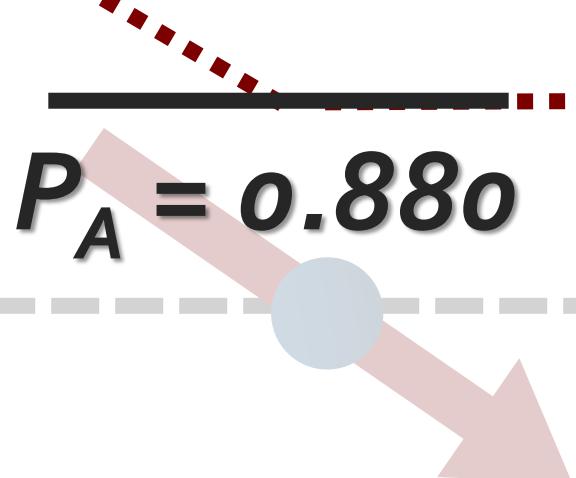
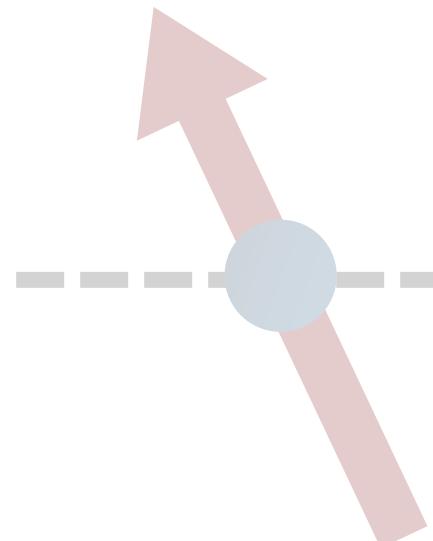
Overview

$P_A = 0.936$

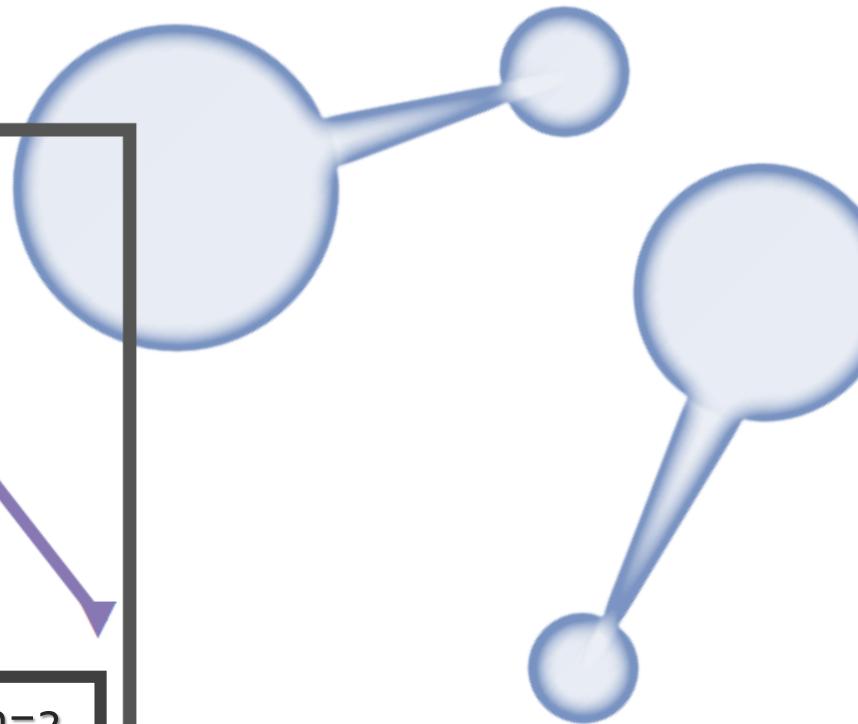
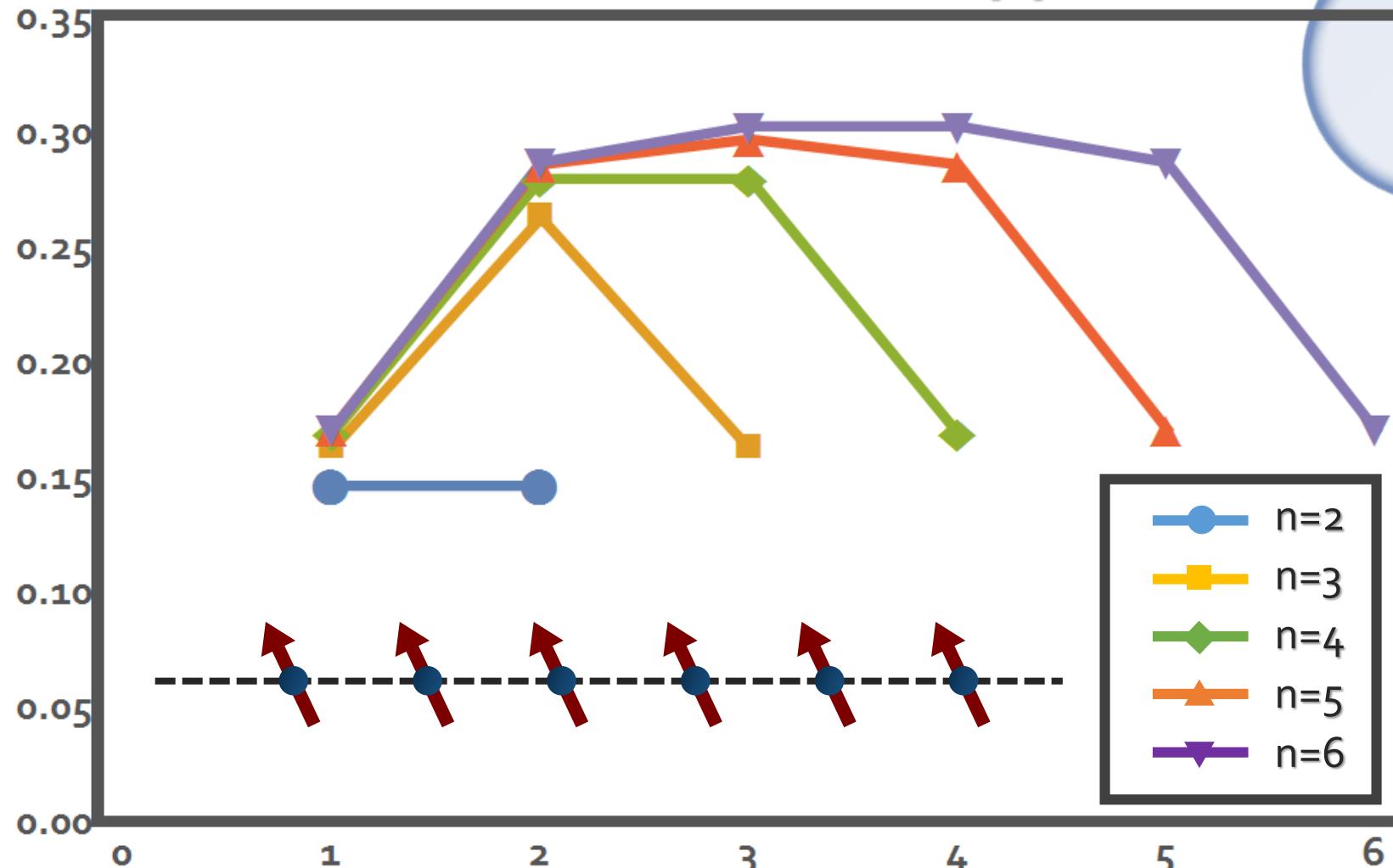
$P_A = 0.880$

$P_A = 0.880$

$P_A = 0.939$



Von Neumann Entropy



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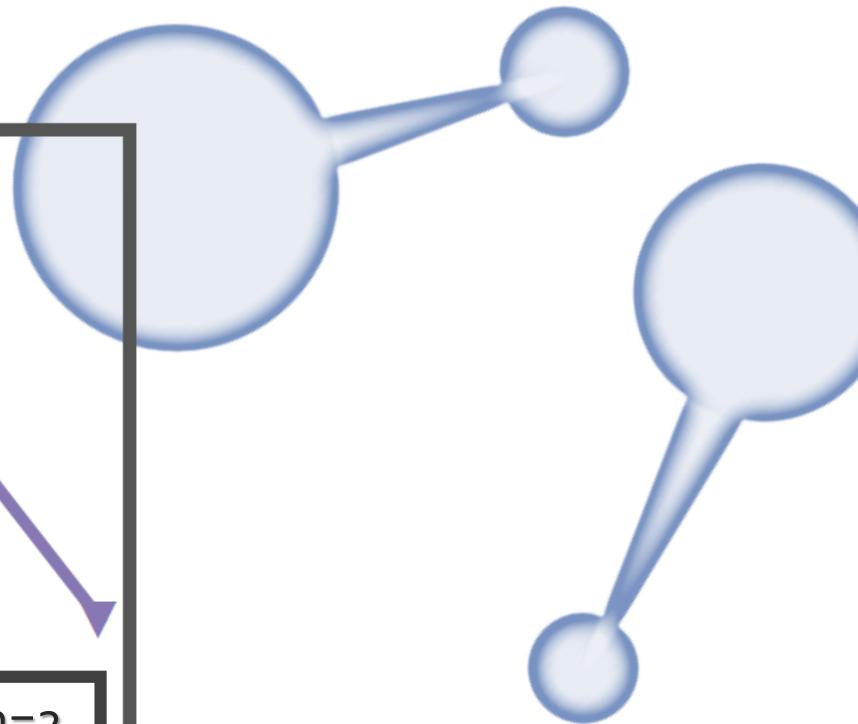
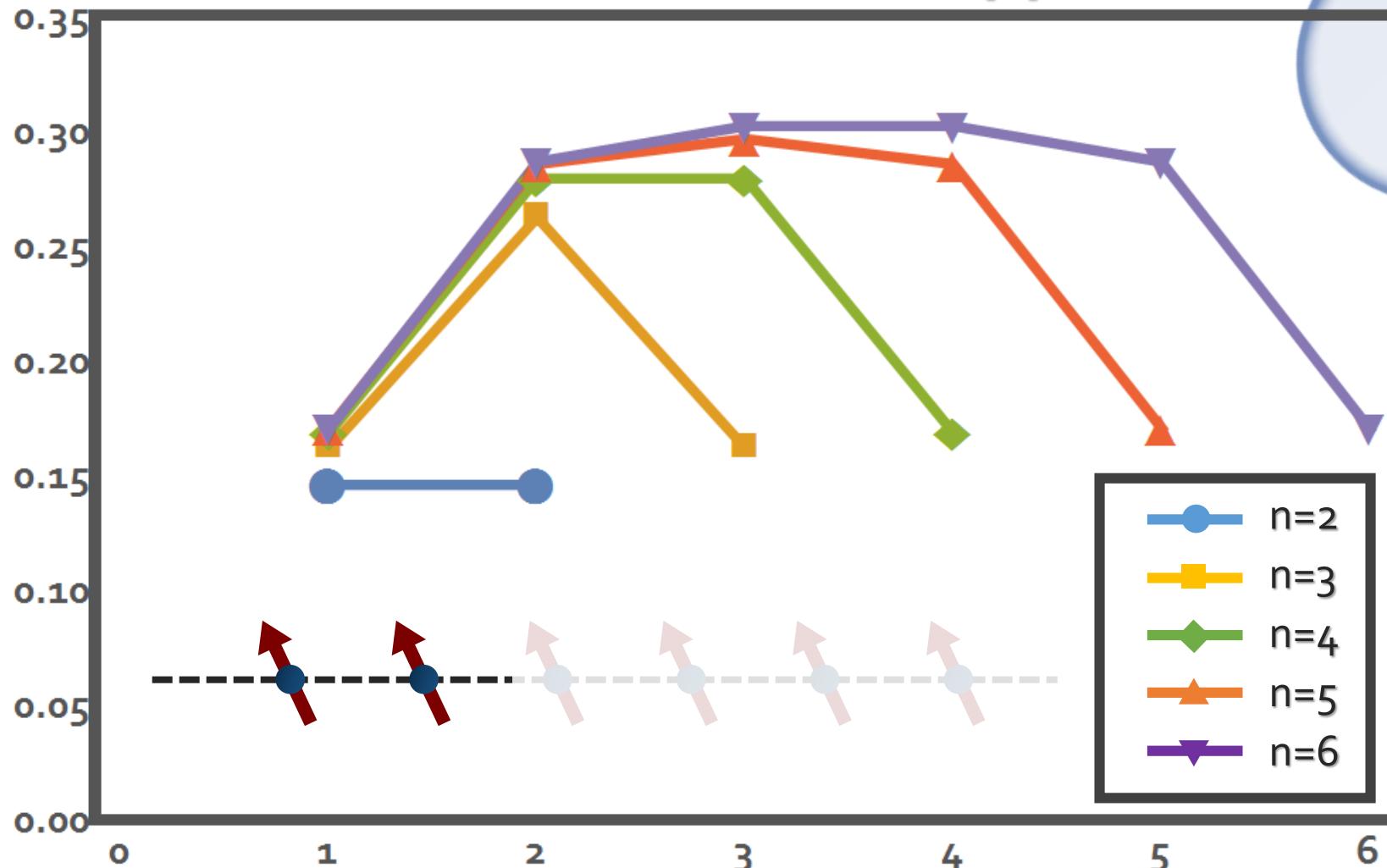
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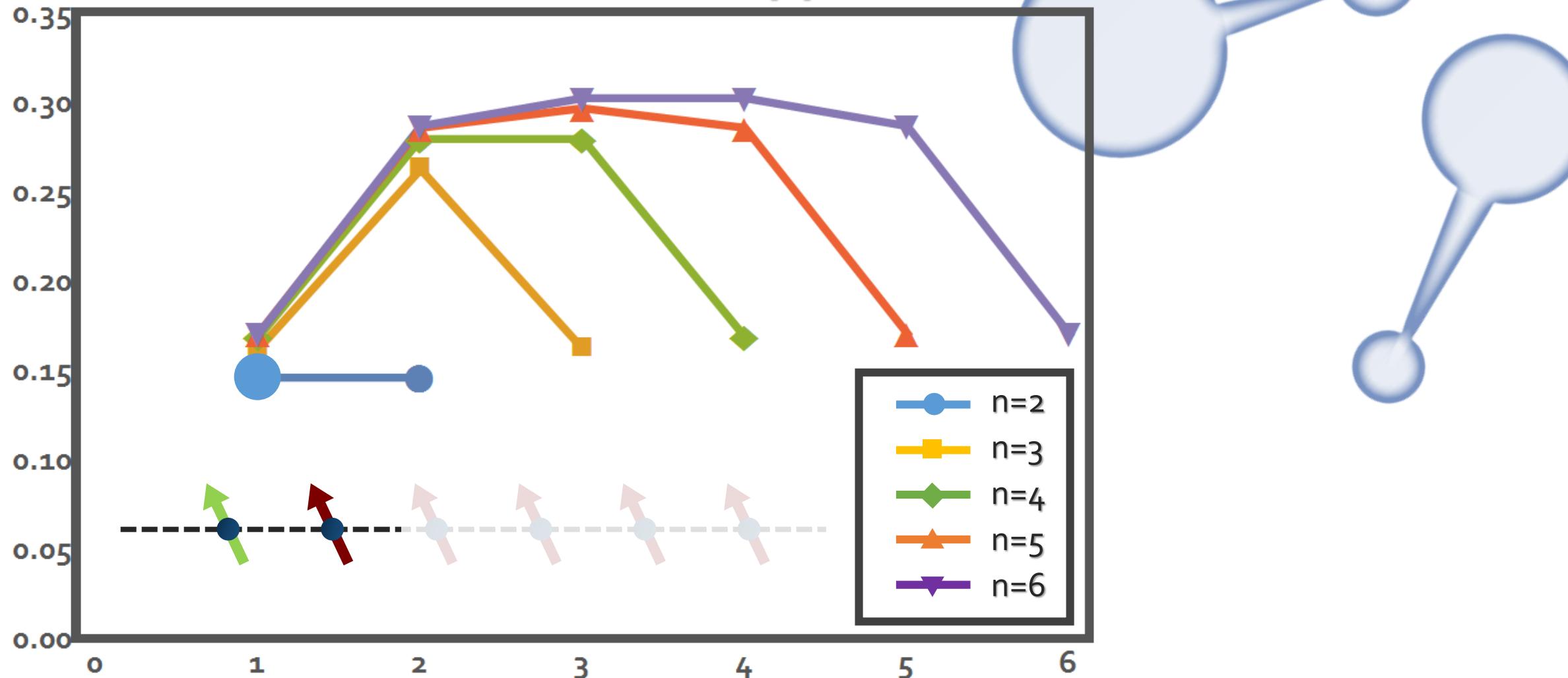
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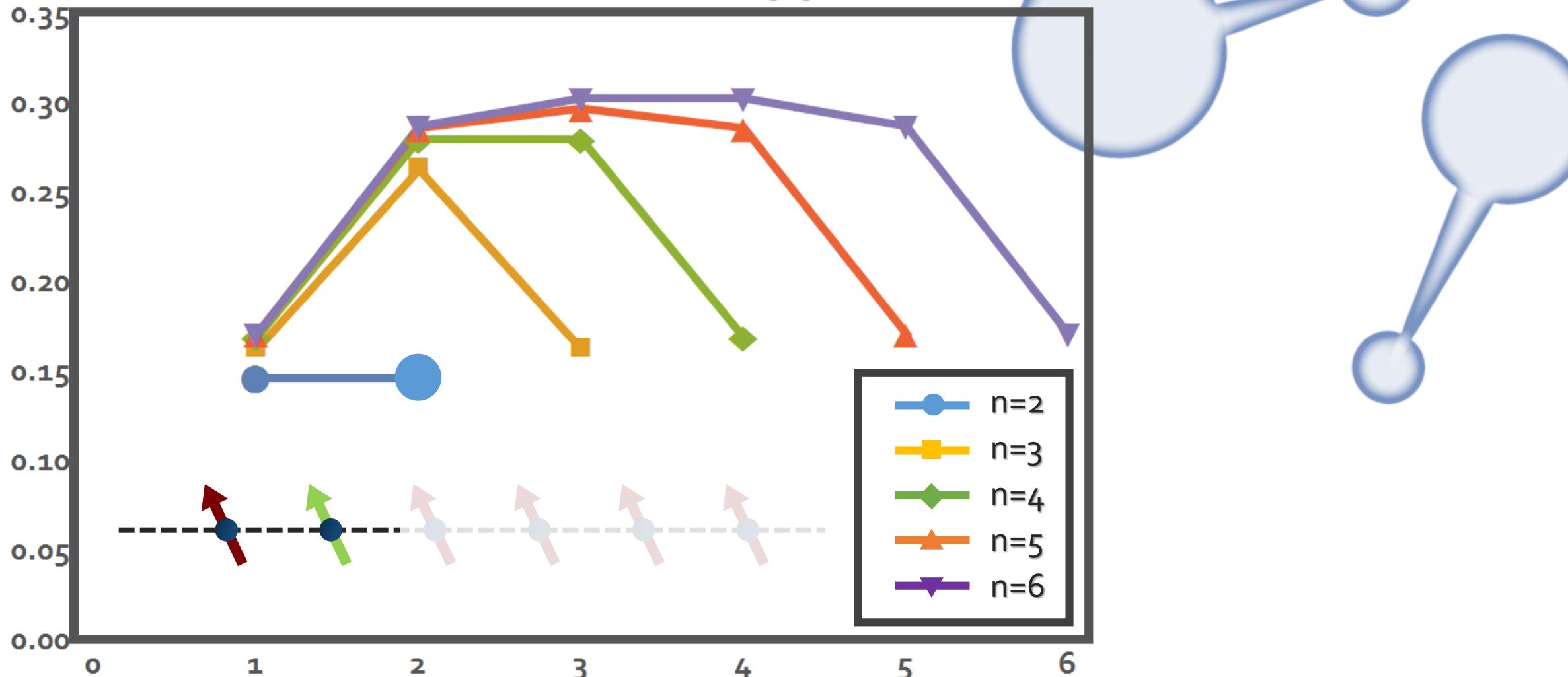
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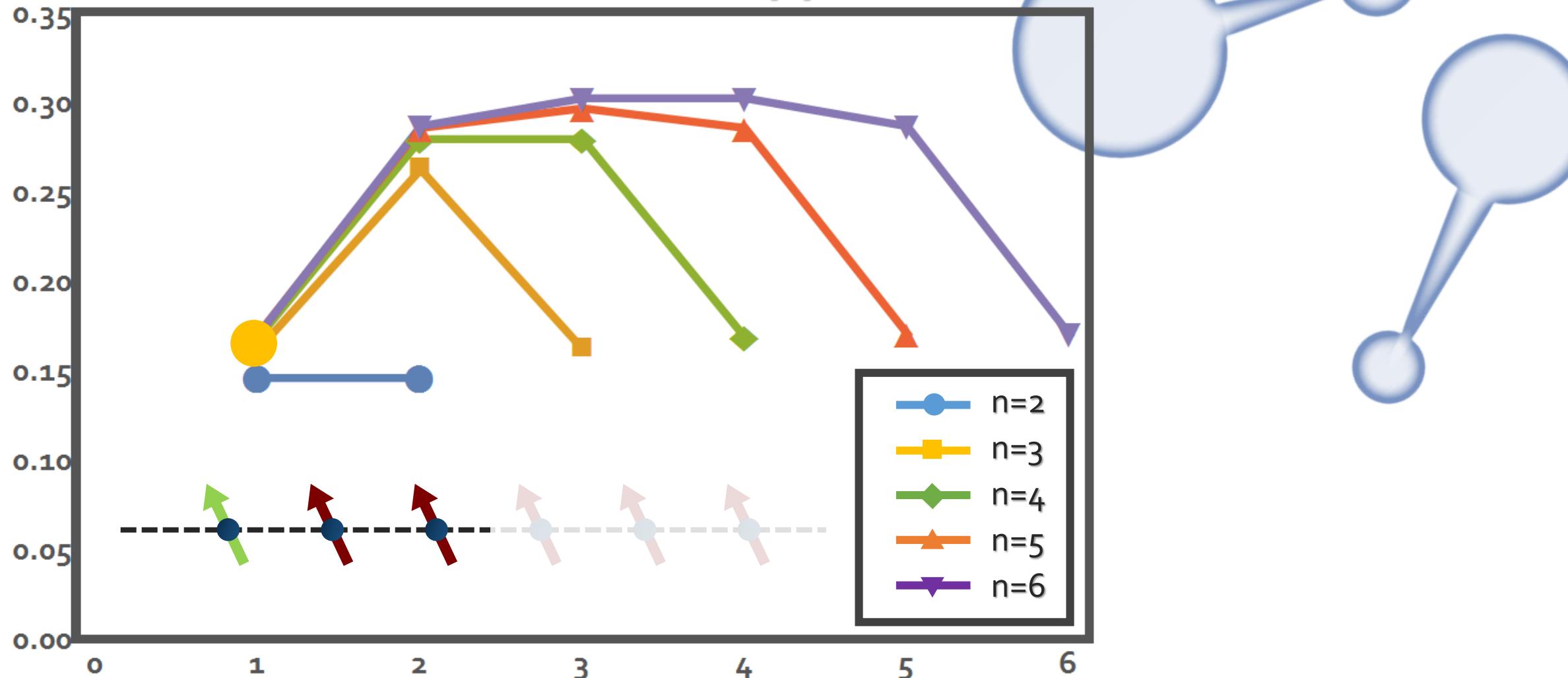
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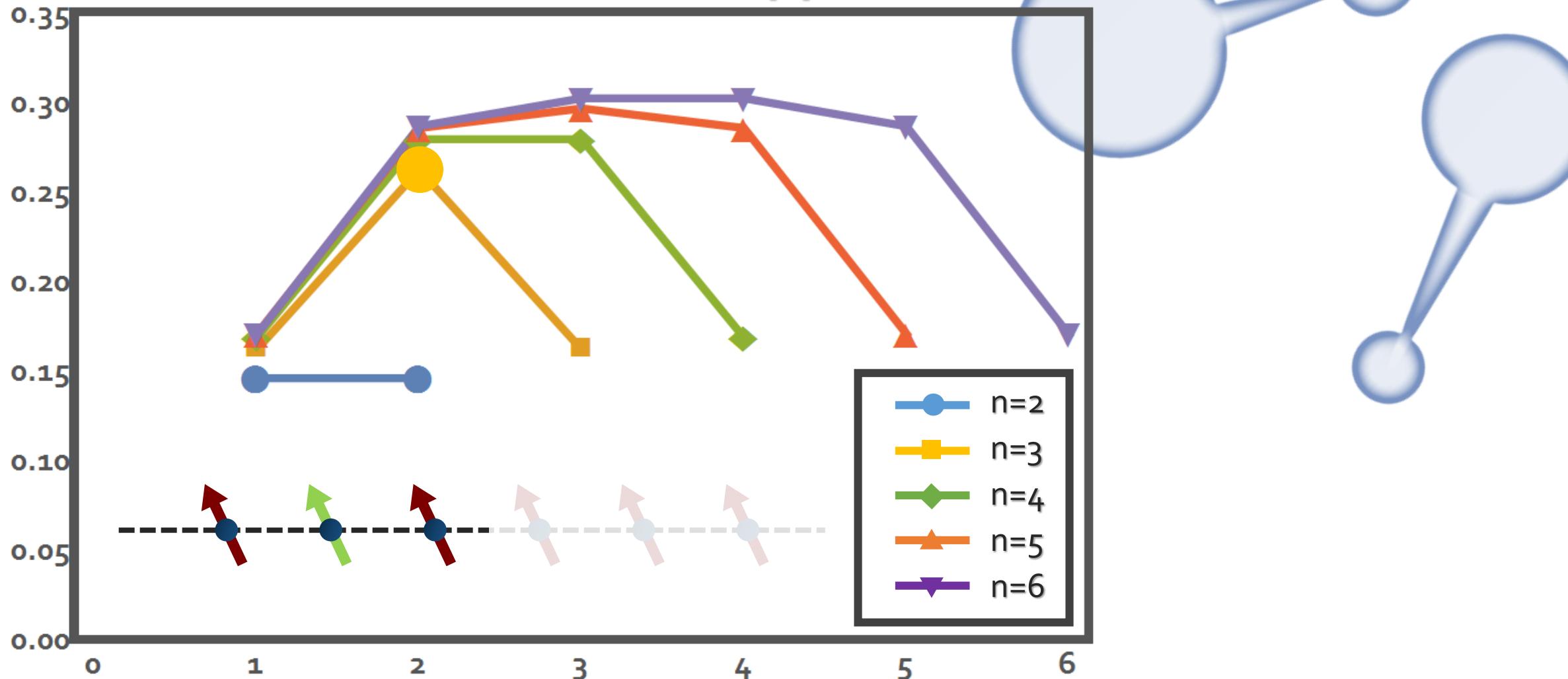
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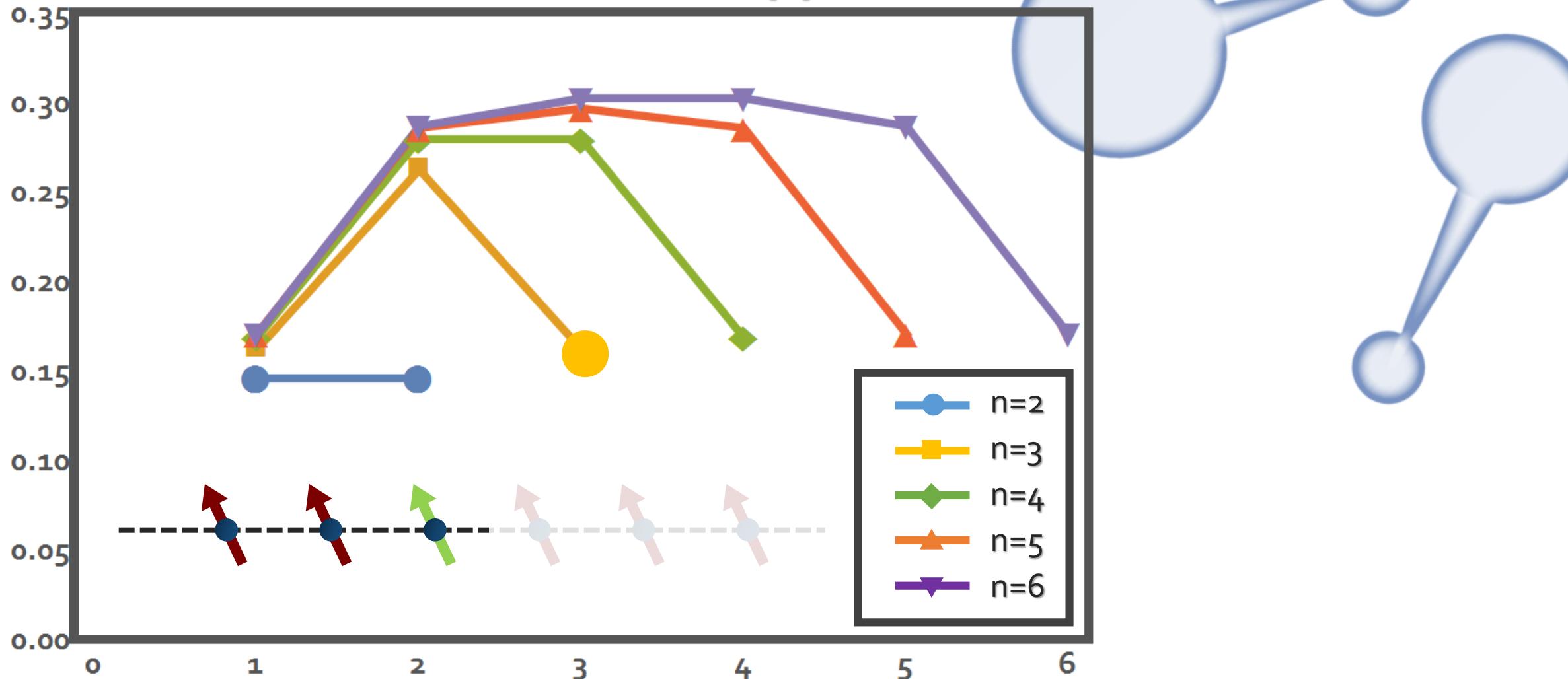
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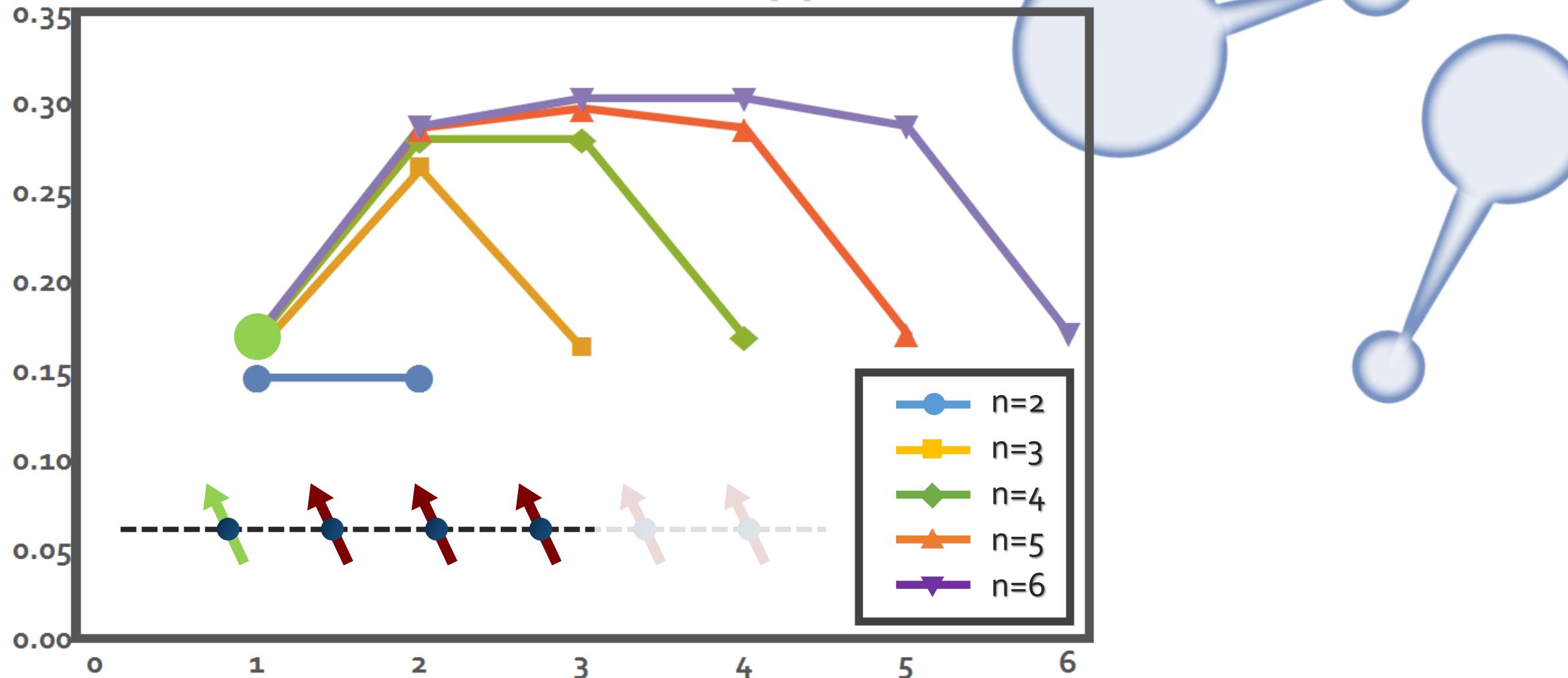
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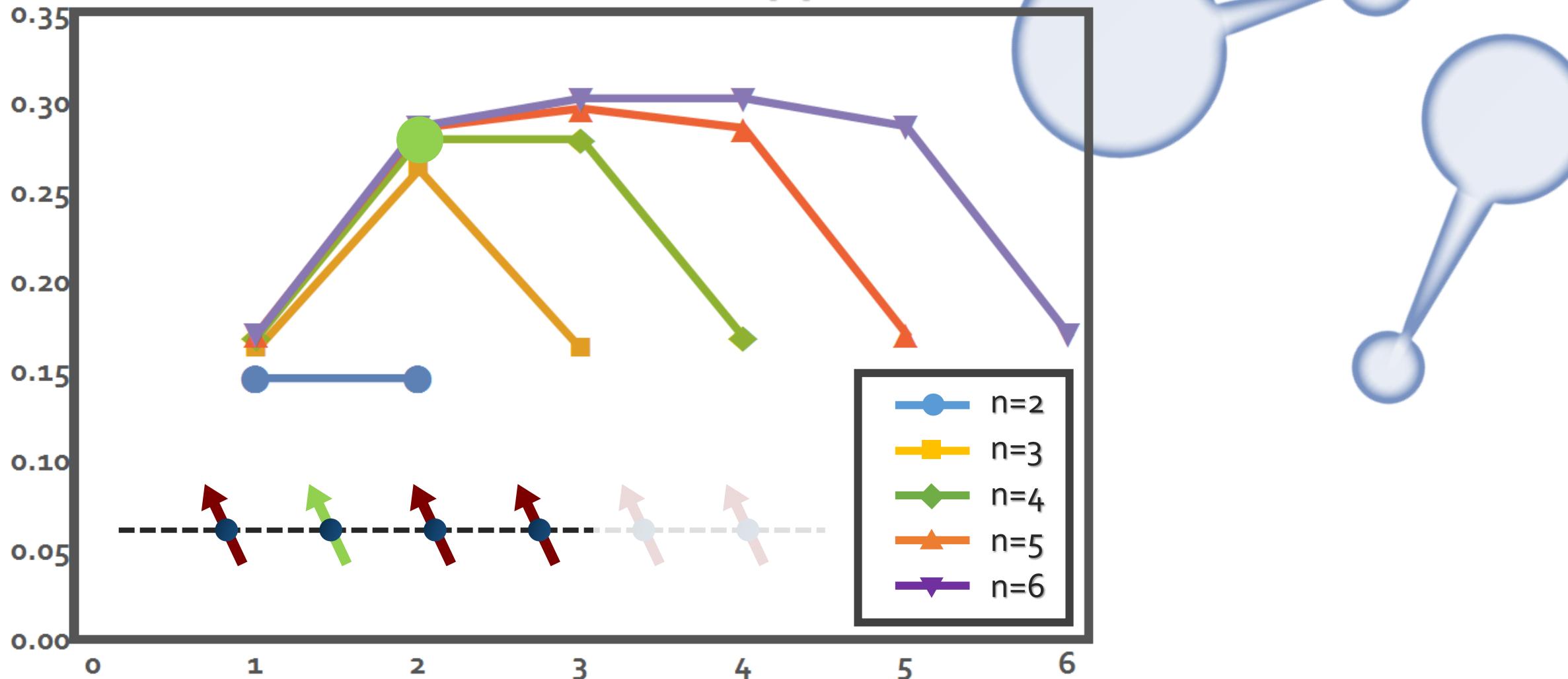
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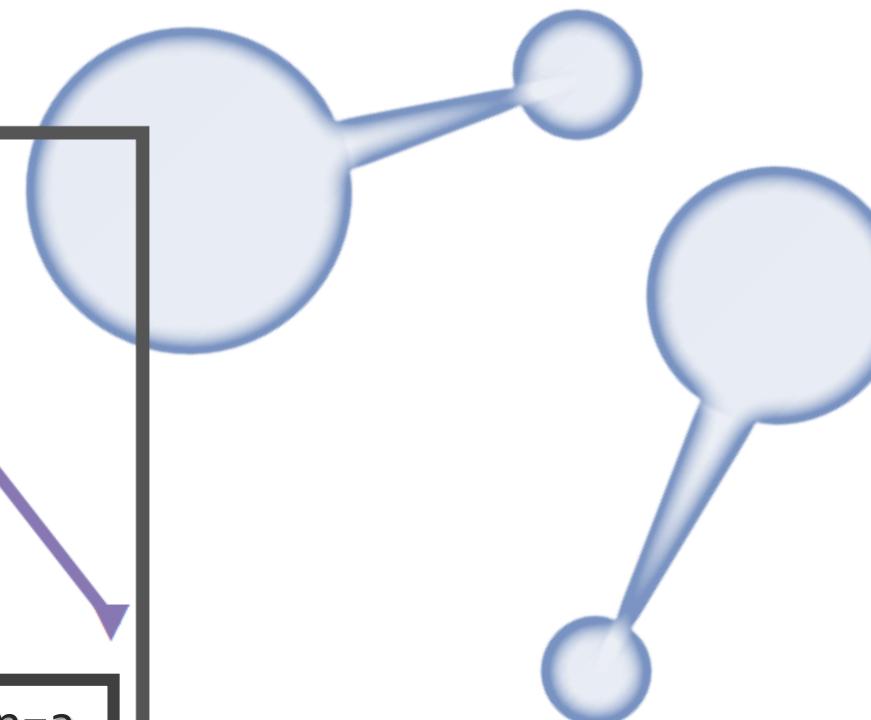
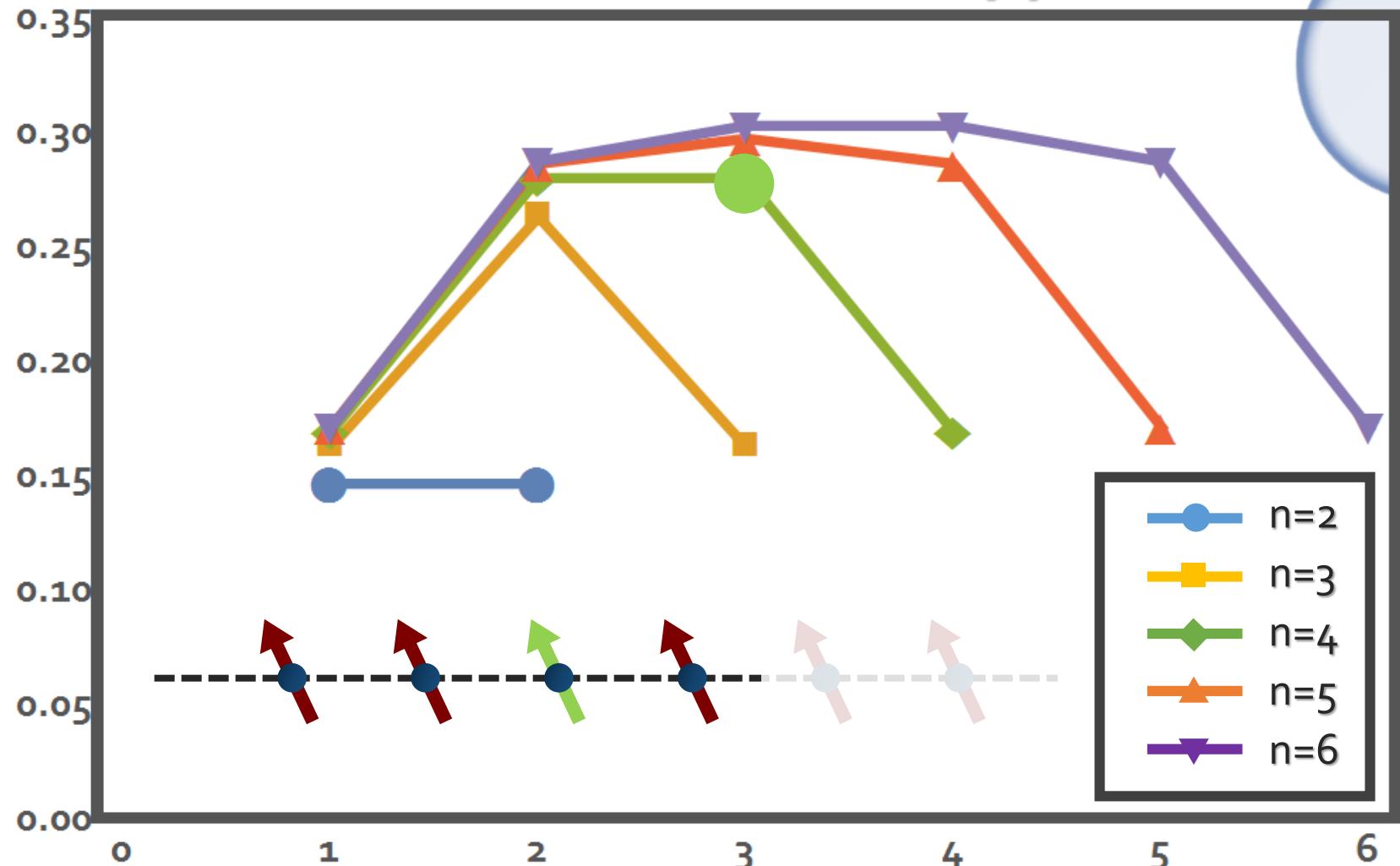
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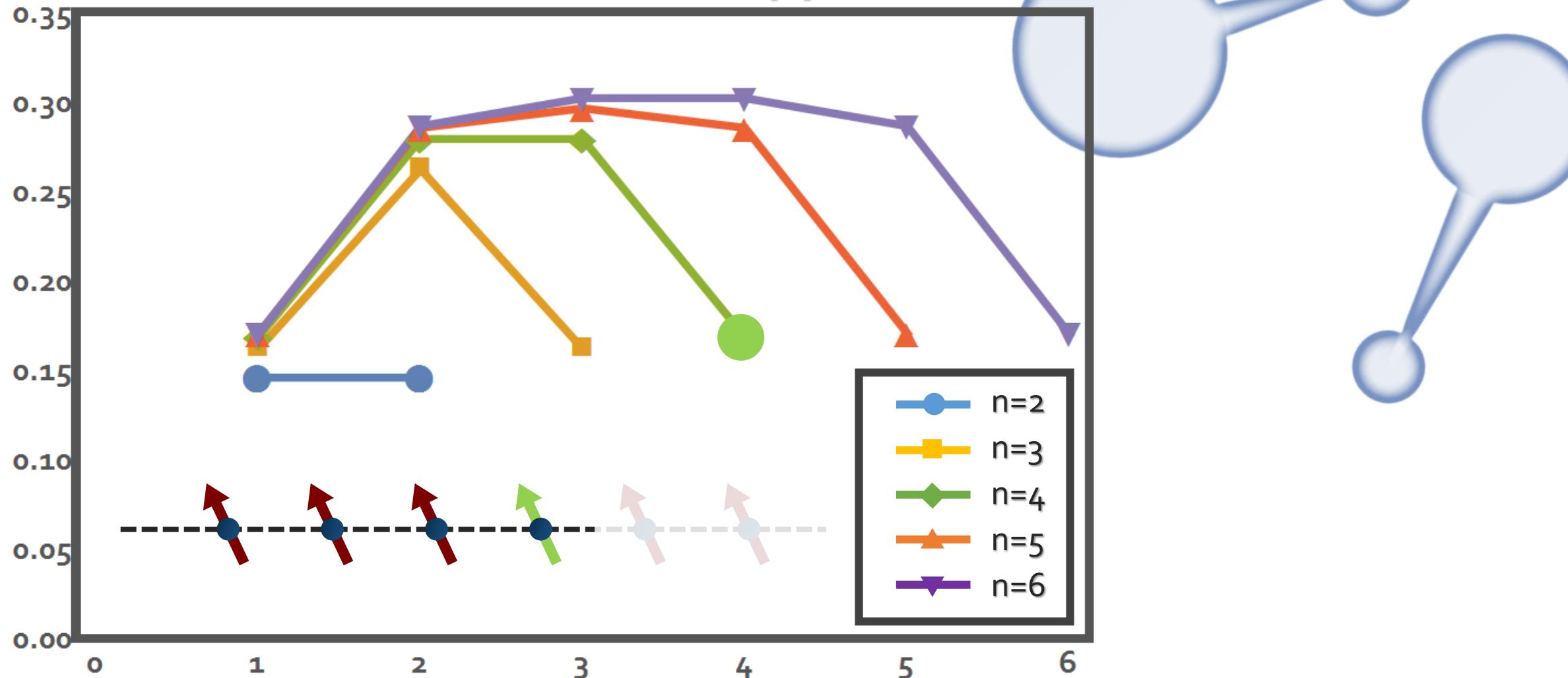
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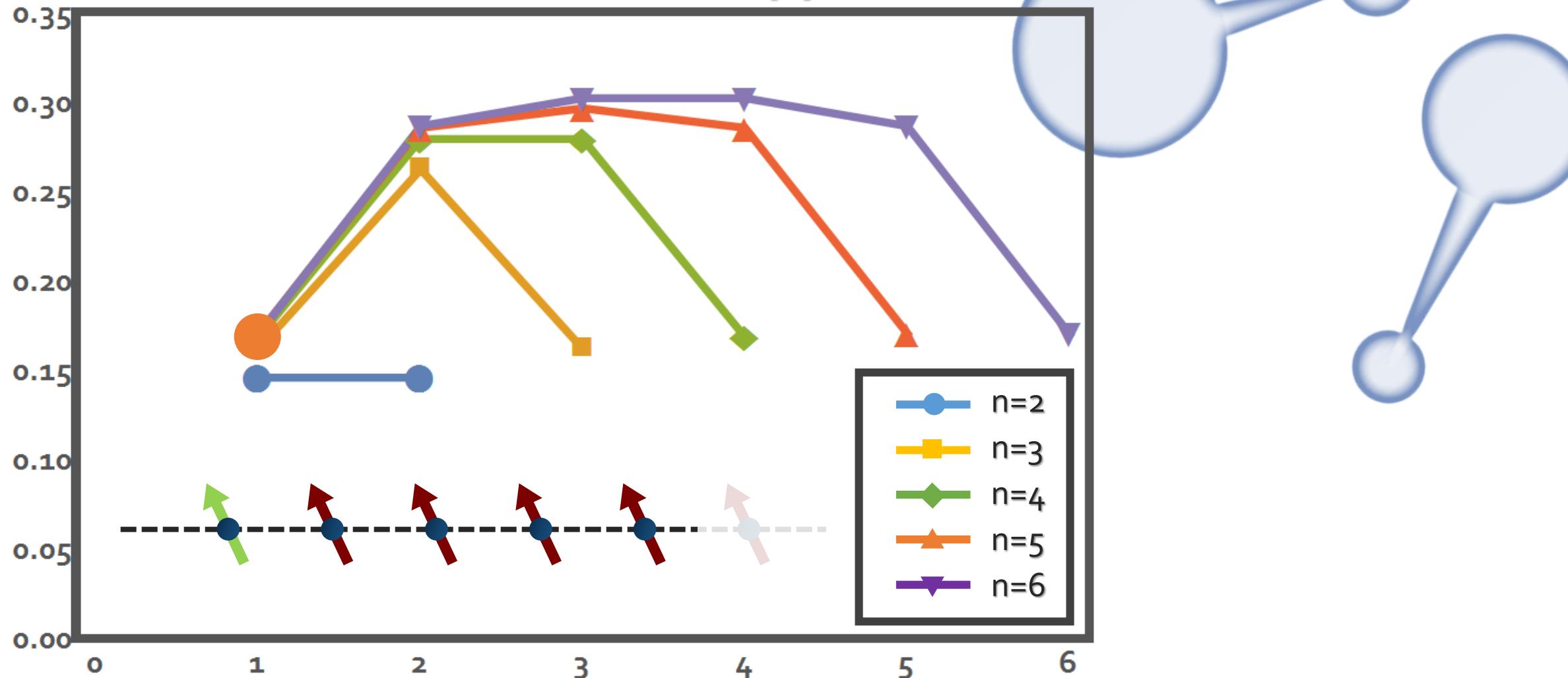
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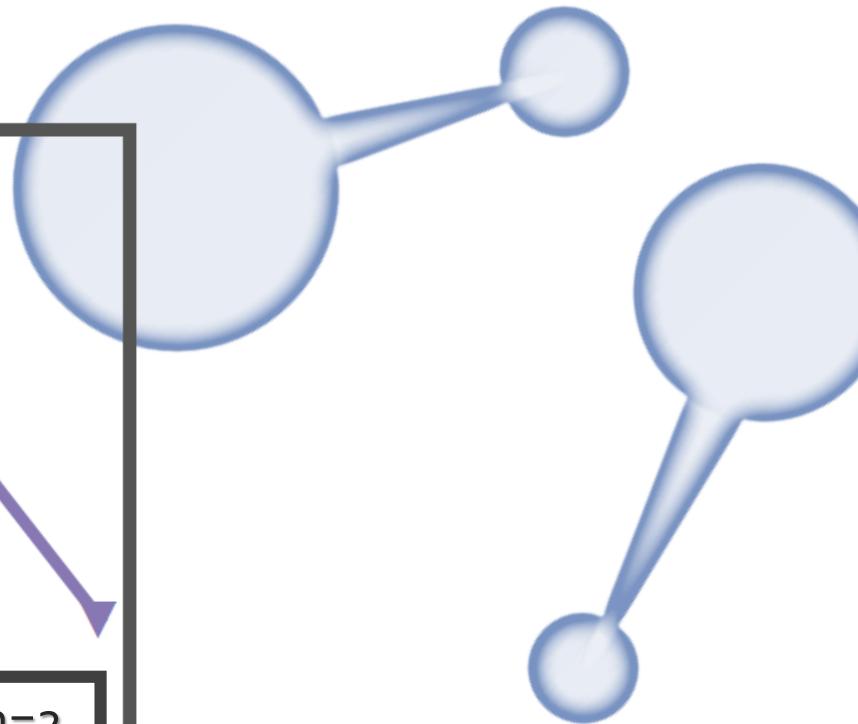
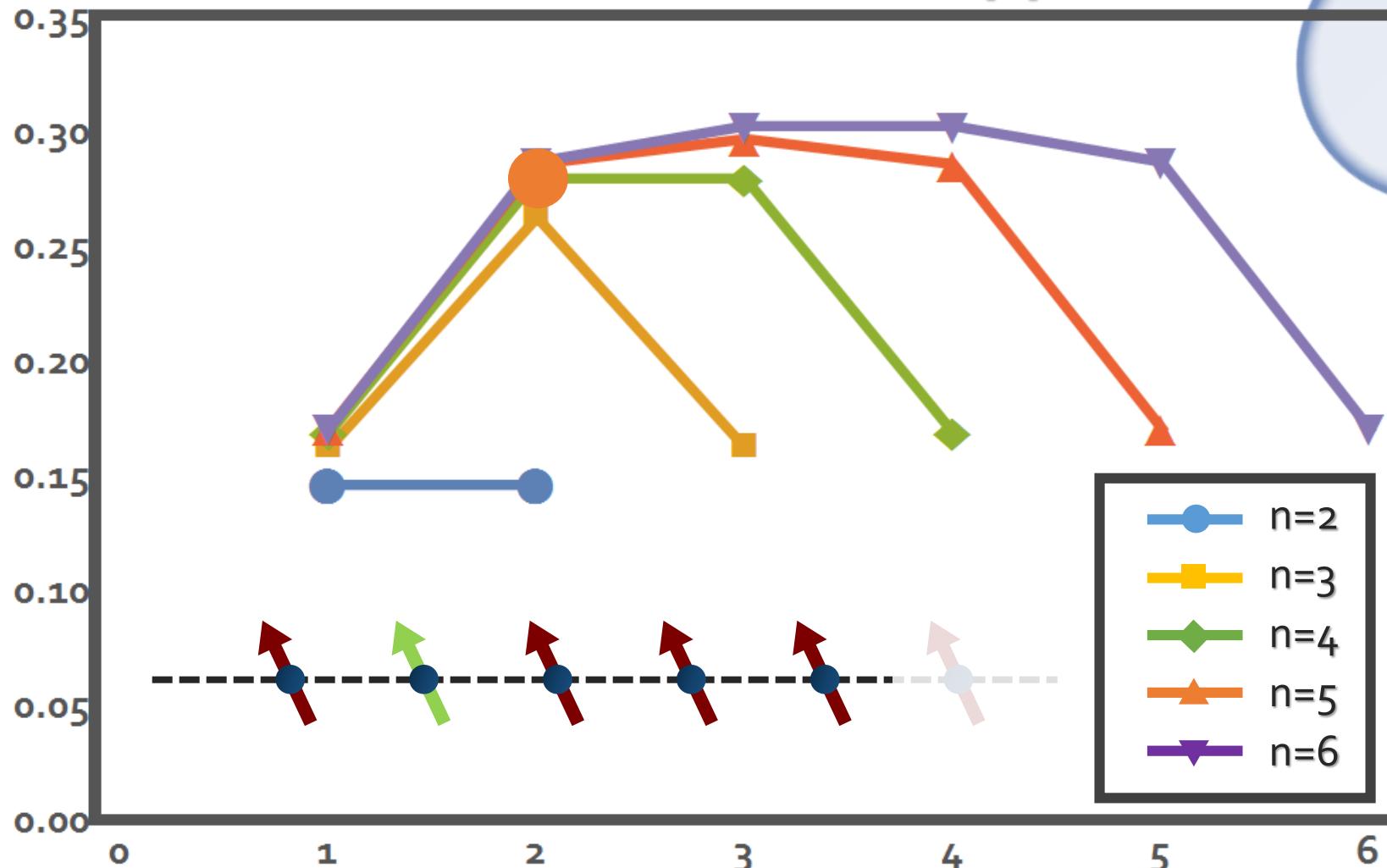
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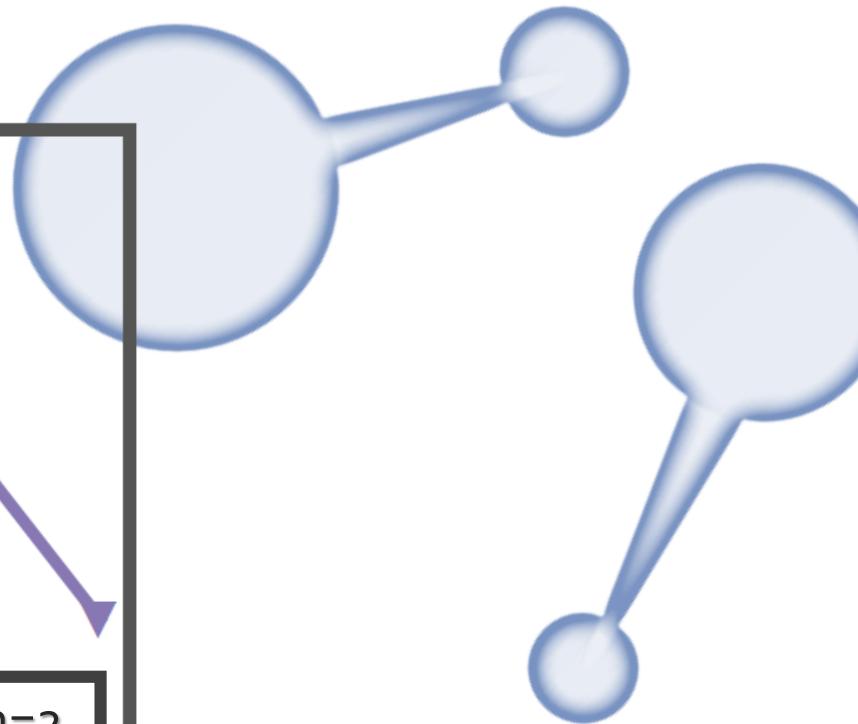
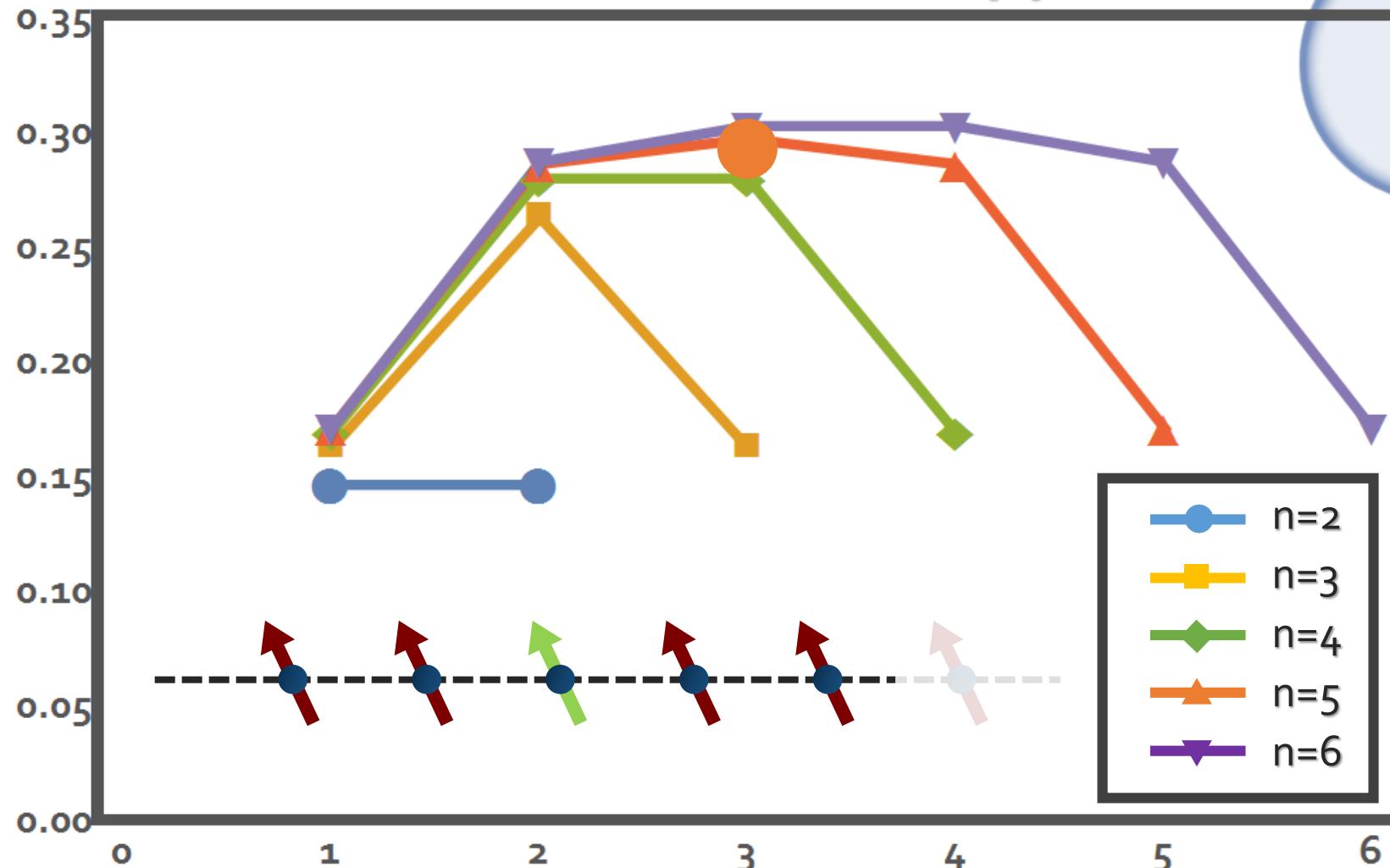
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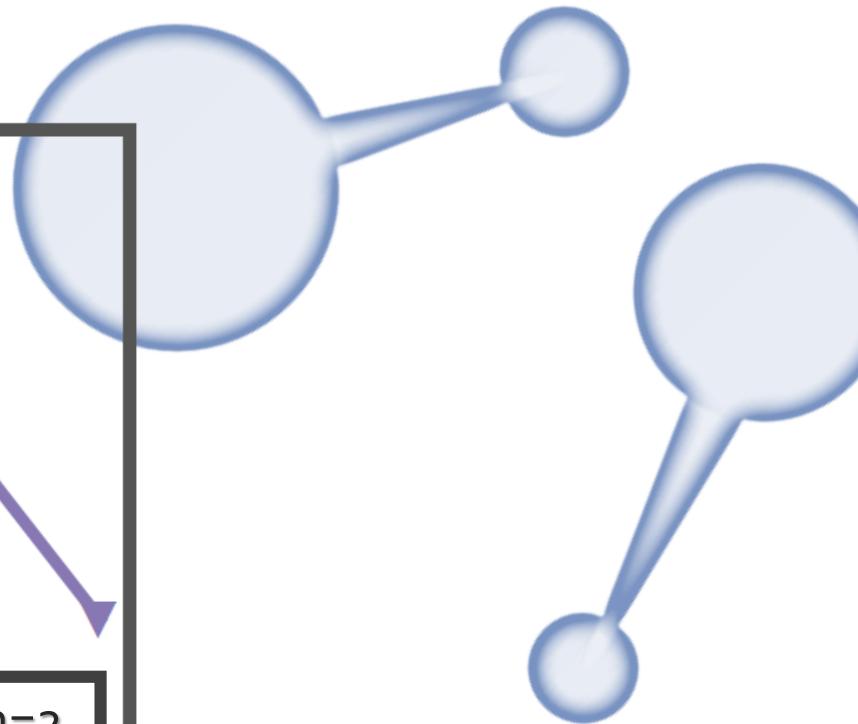
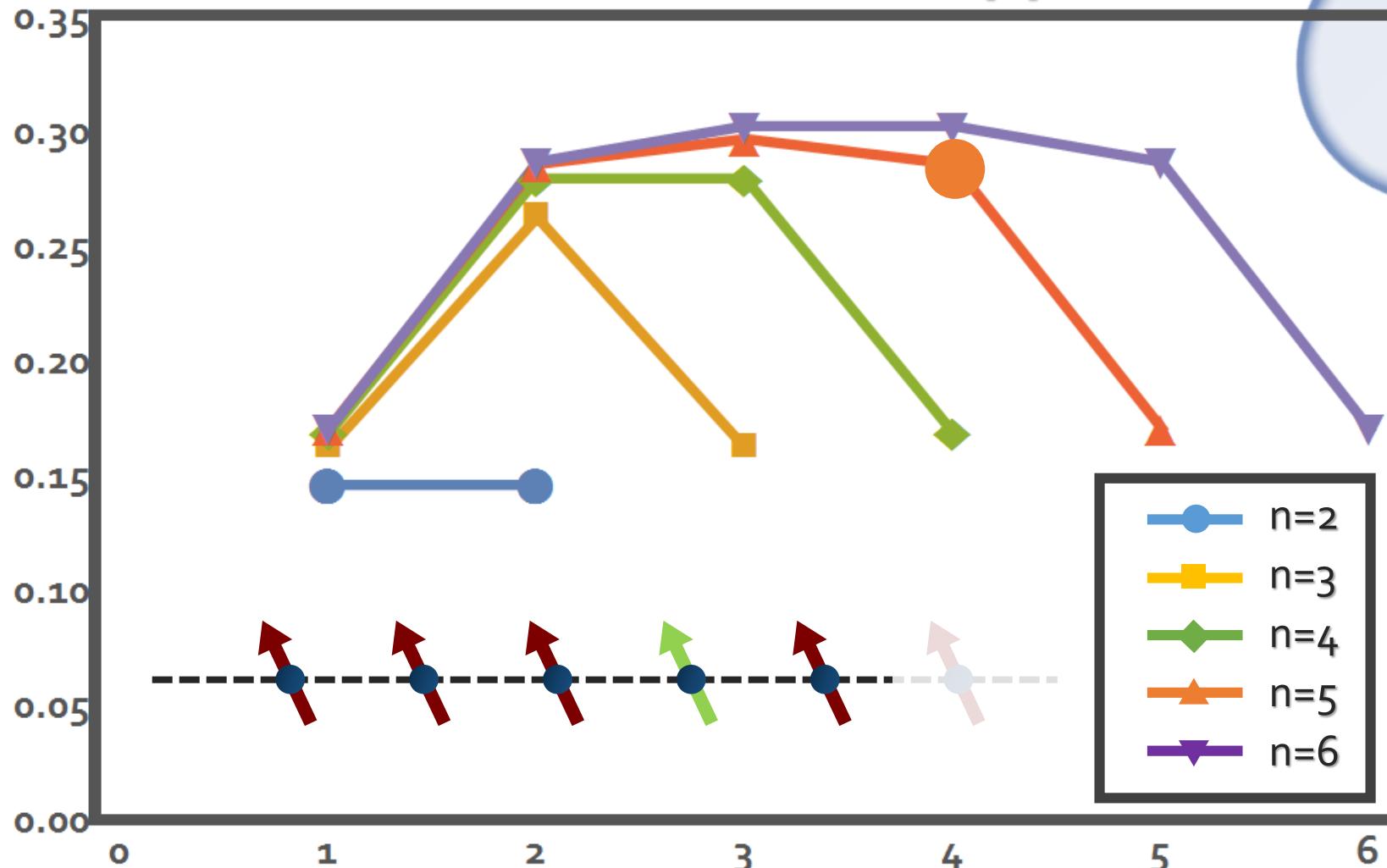
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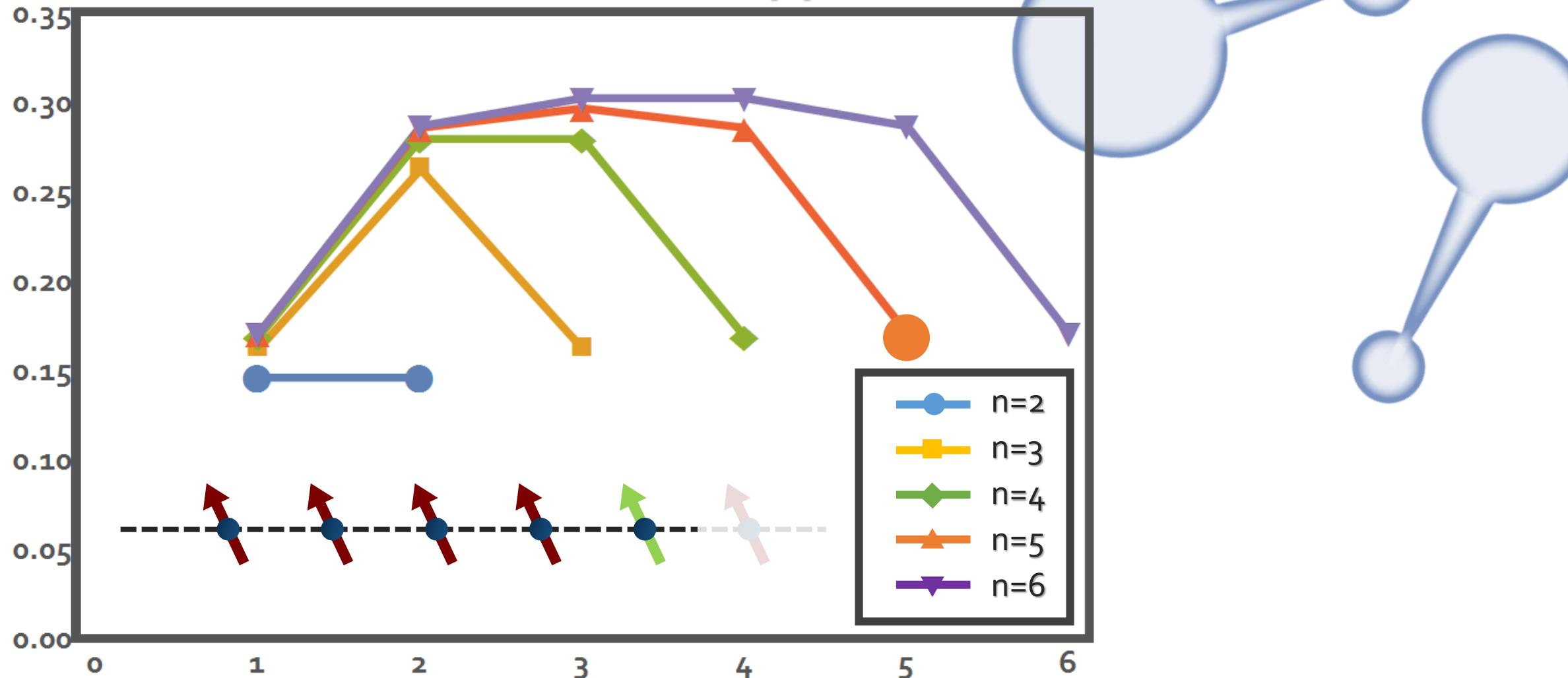
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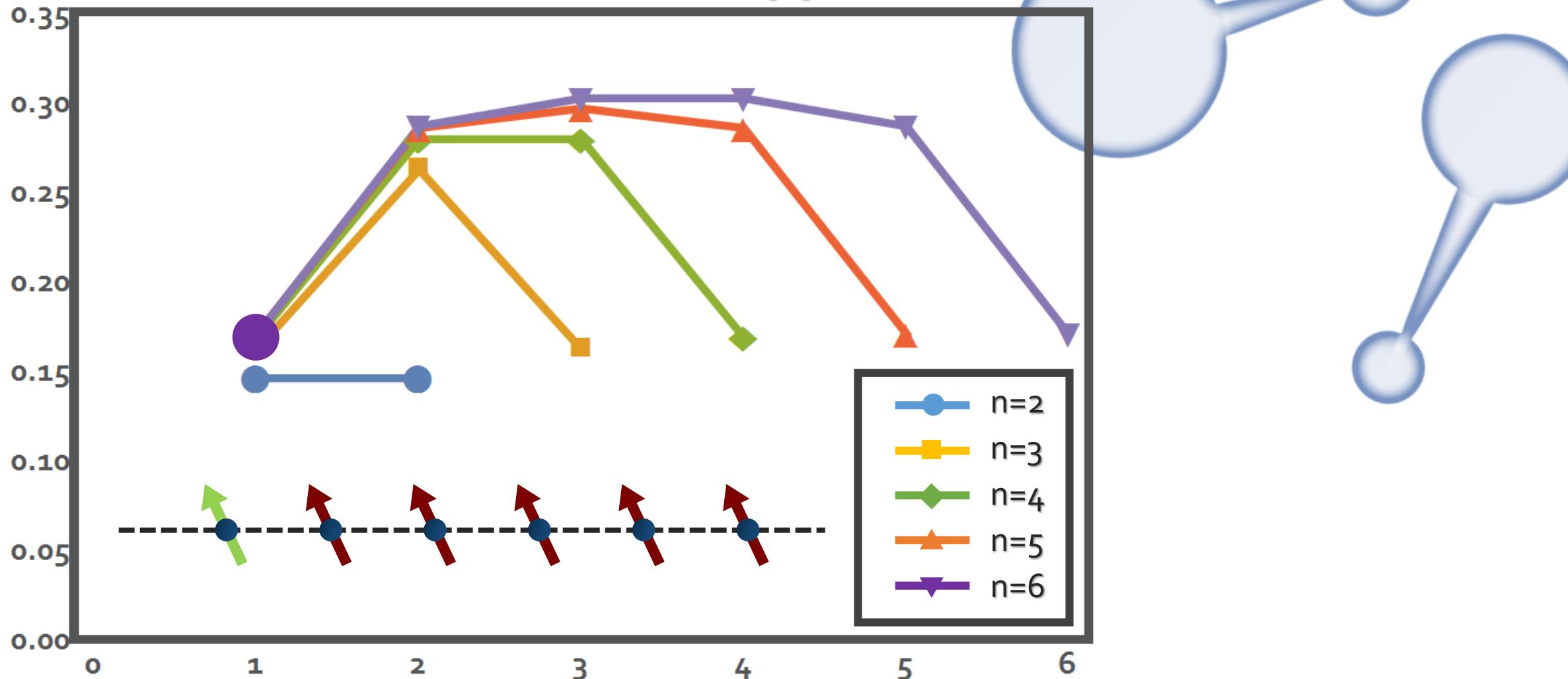
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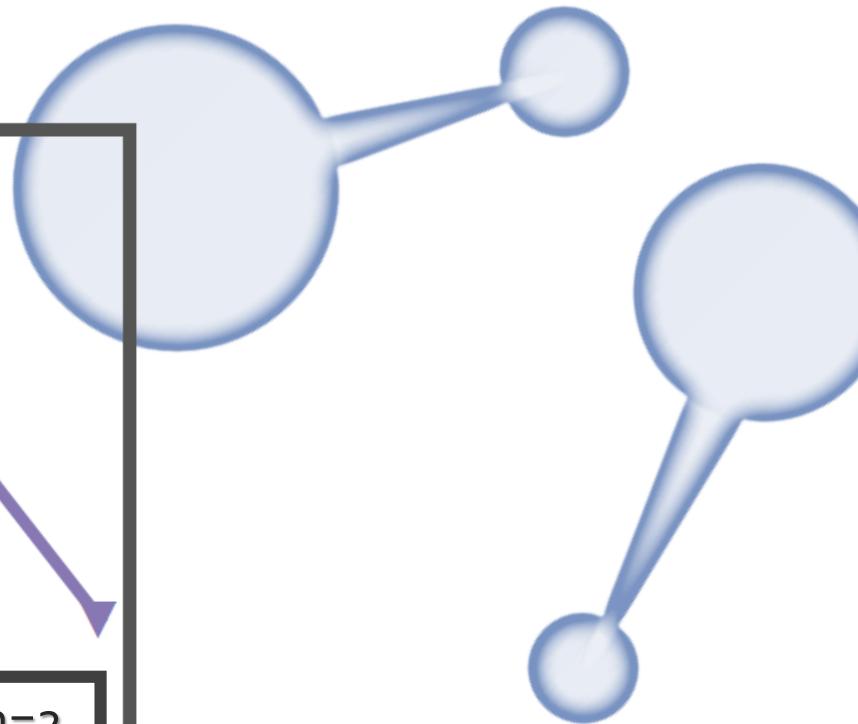
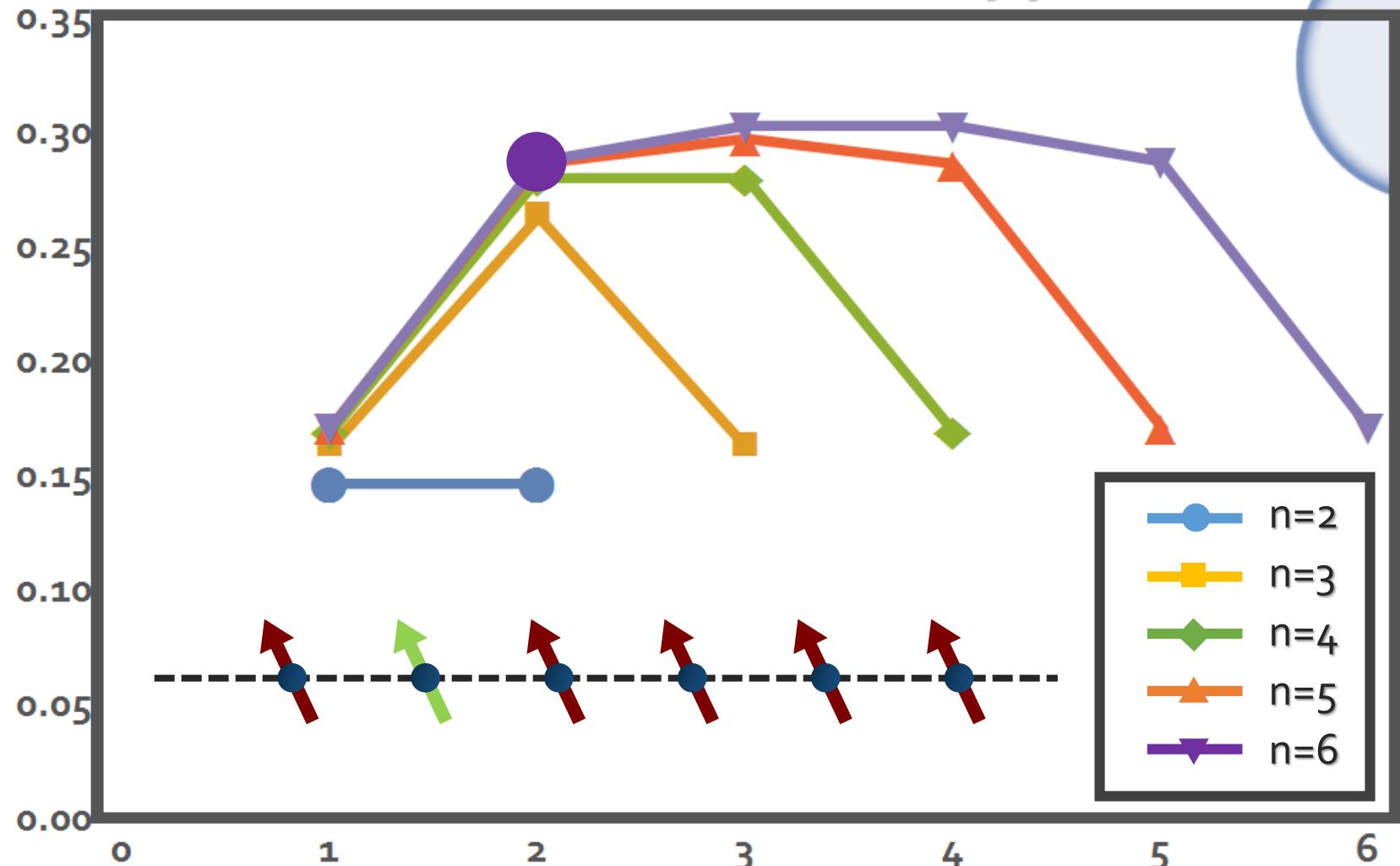
Confined Water

Dipole Chains

Hydrogen Clusters

Overview

Von Neumann Entropy



Conclusions

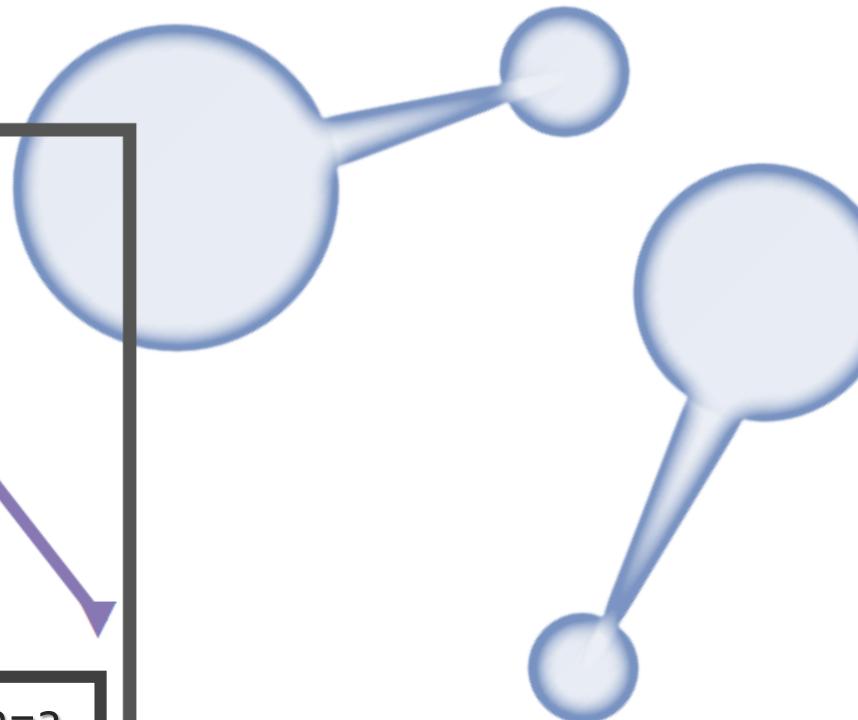
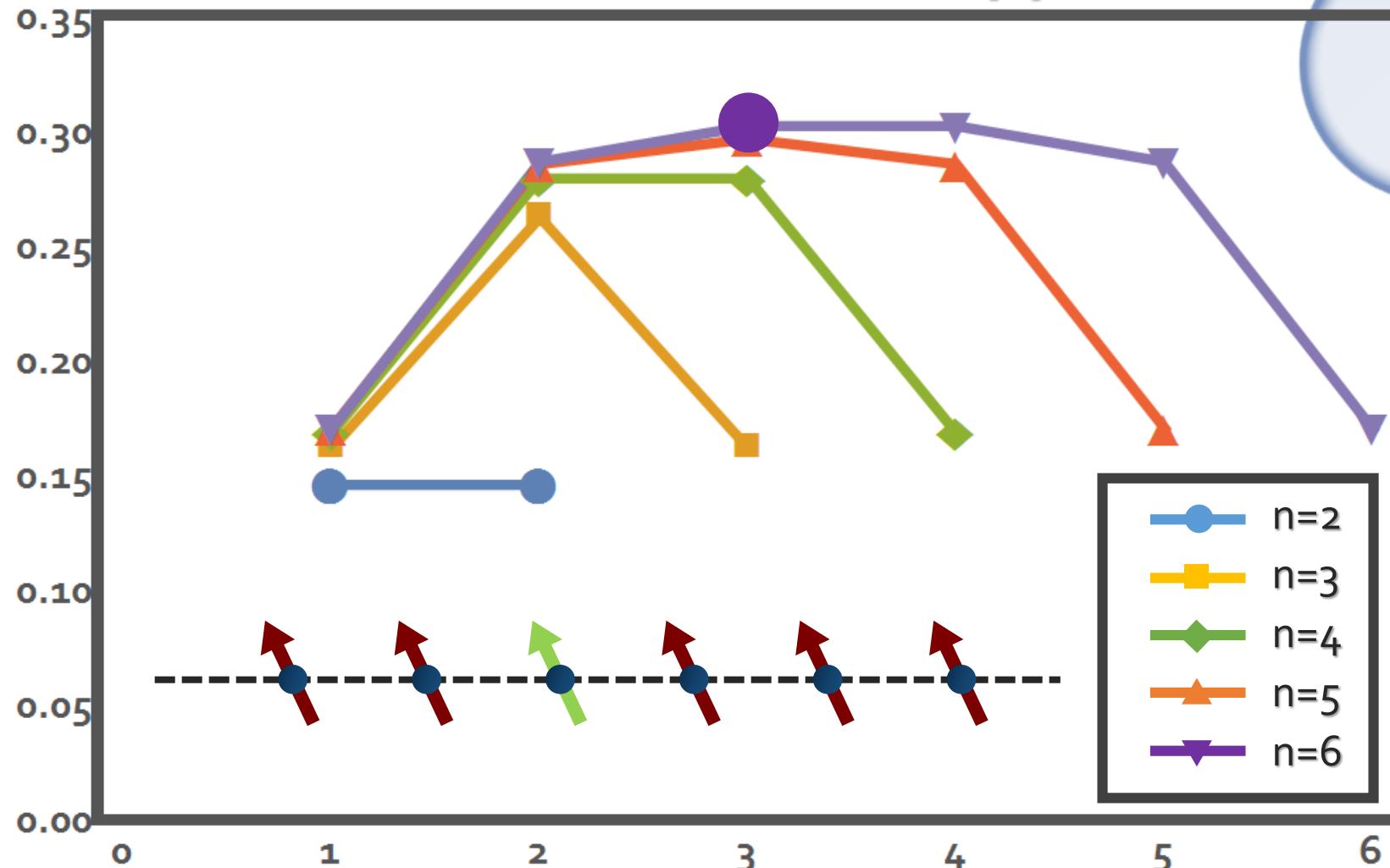
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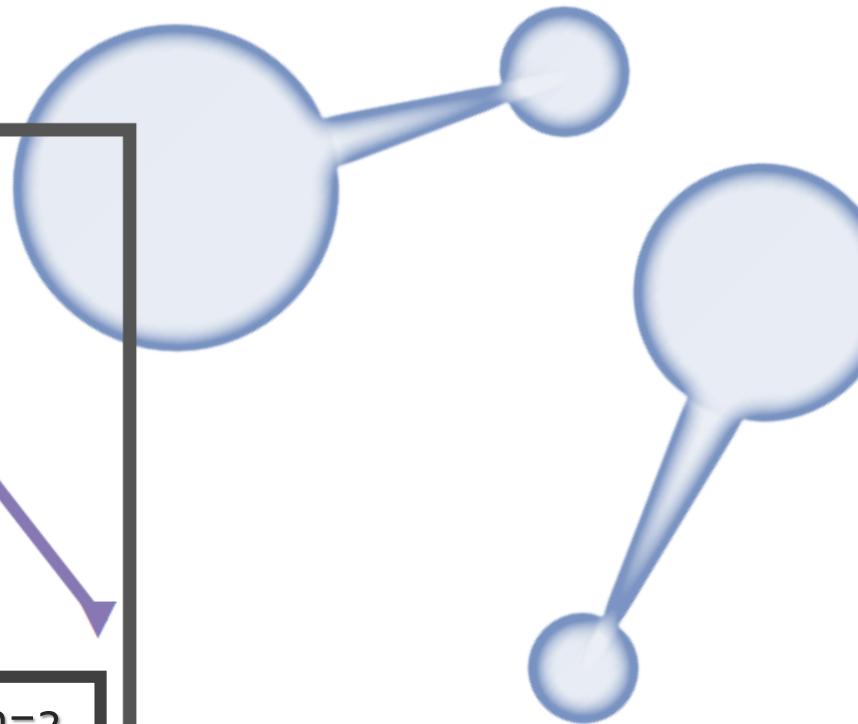
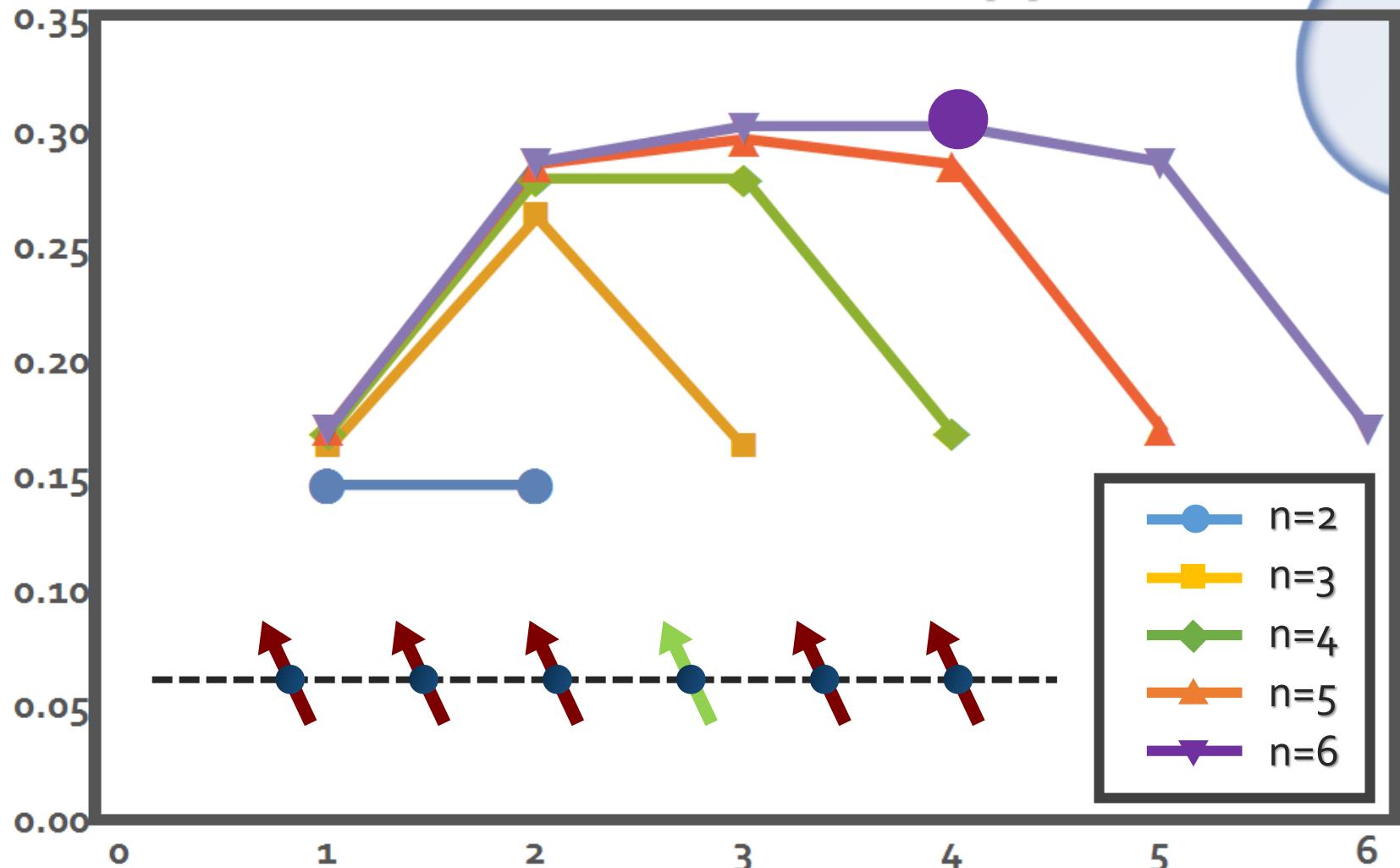
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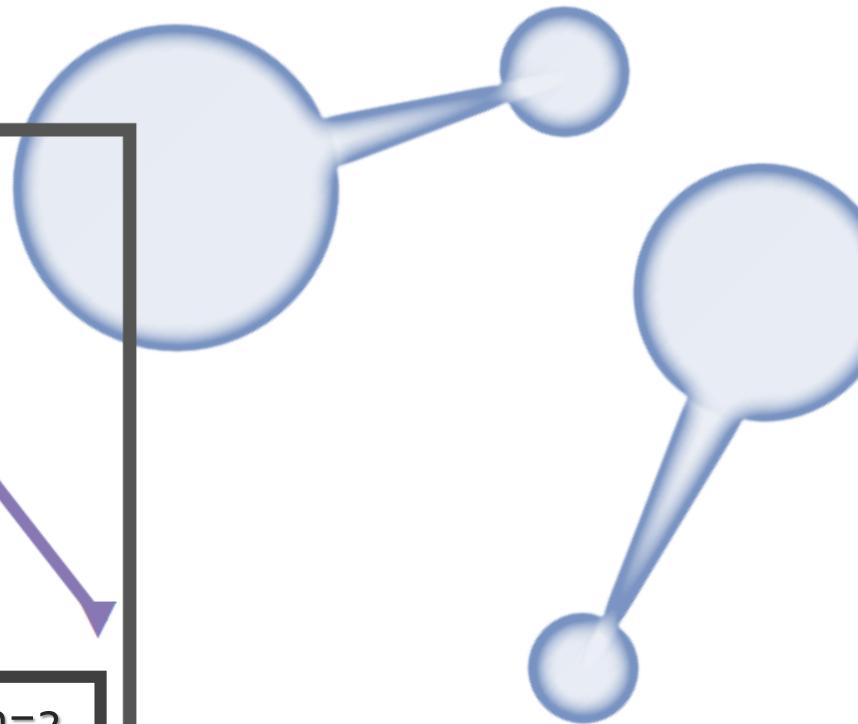
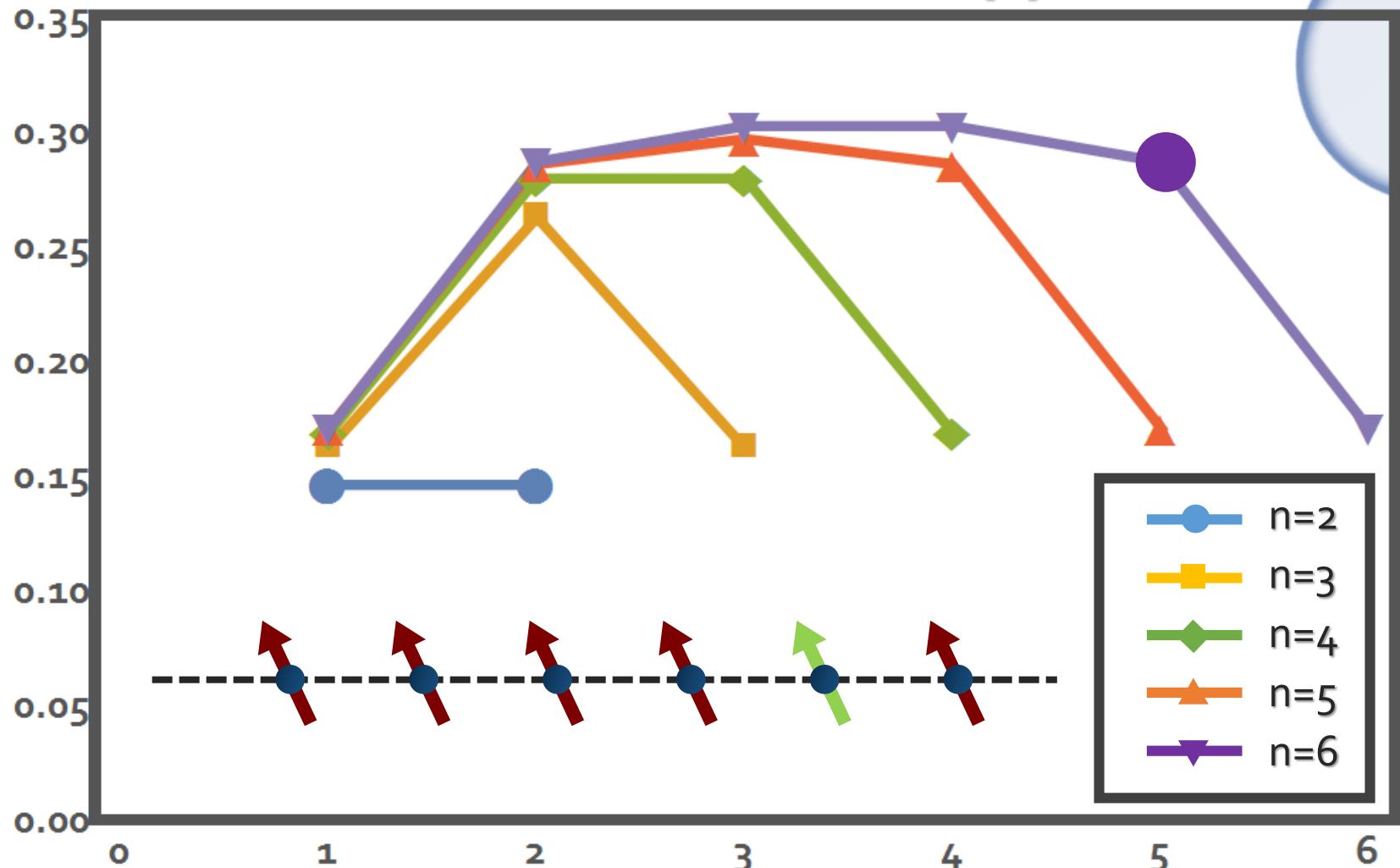
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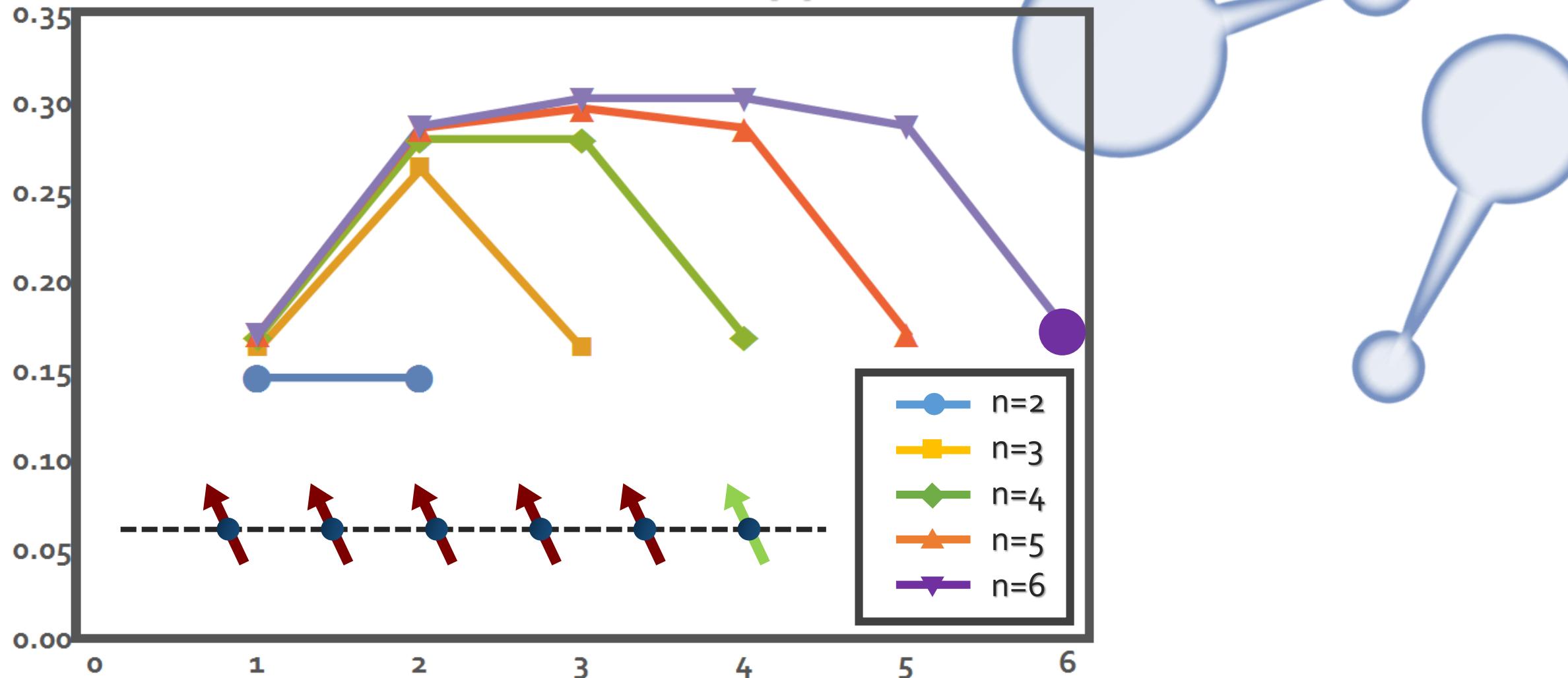
Confined Water

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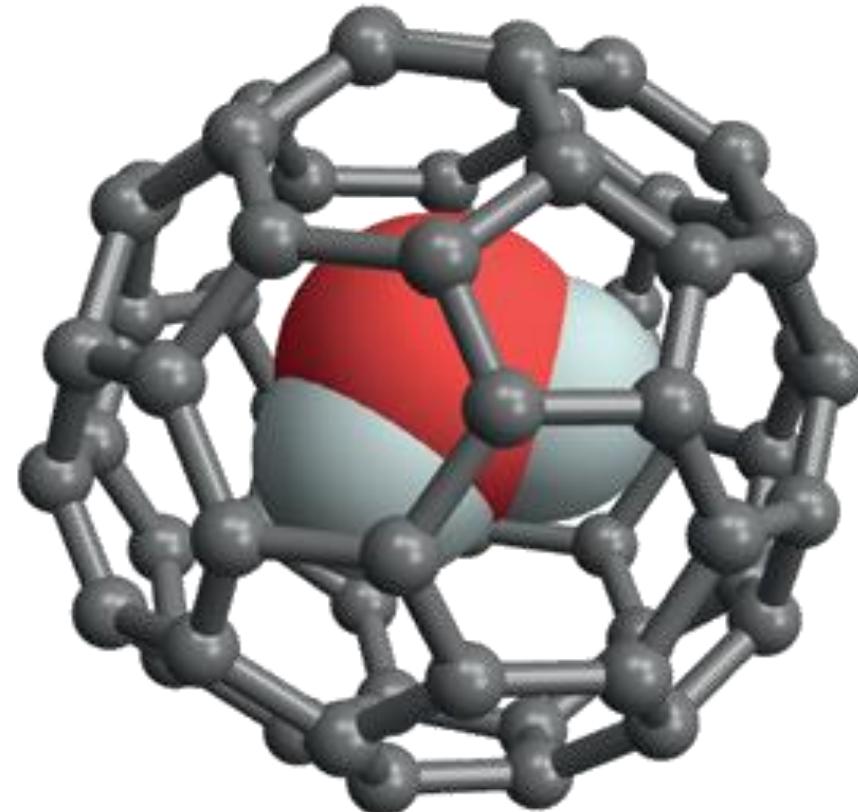
Hydrogen Clusters

Overview

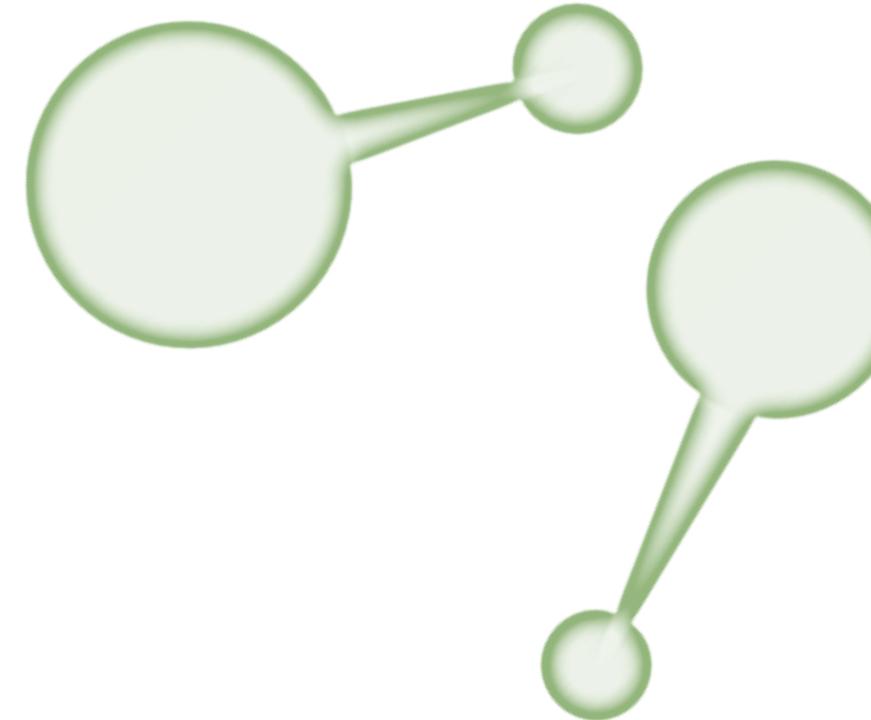
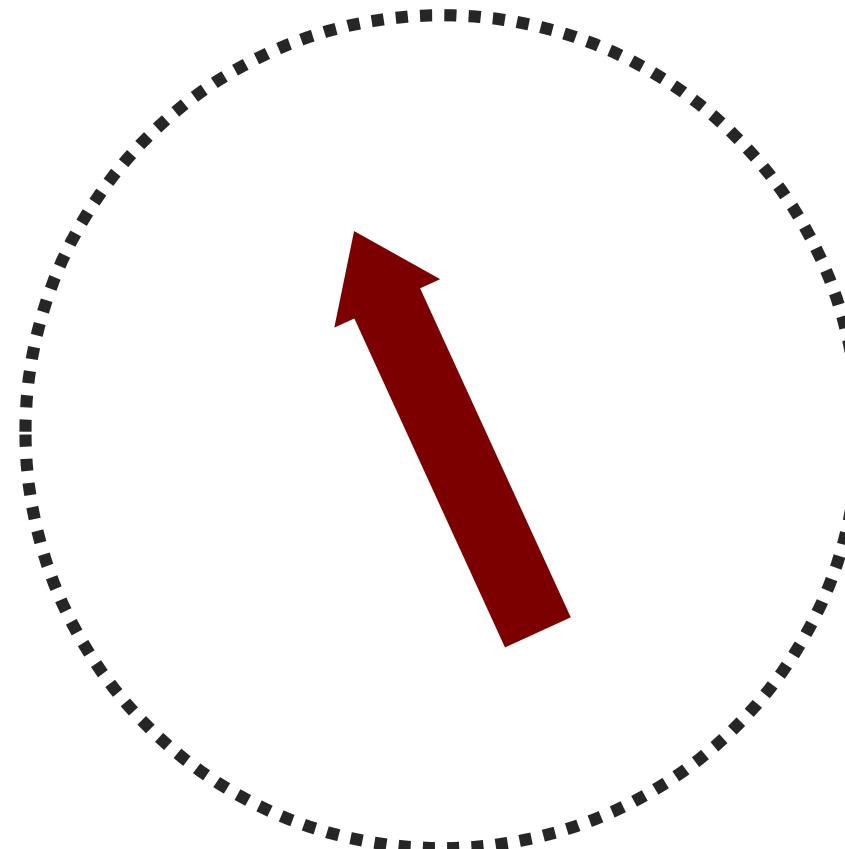


What is next?

Confinement

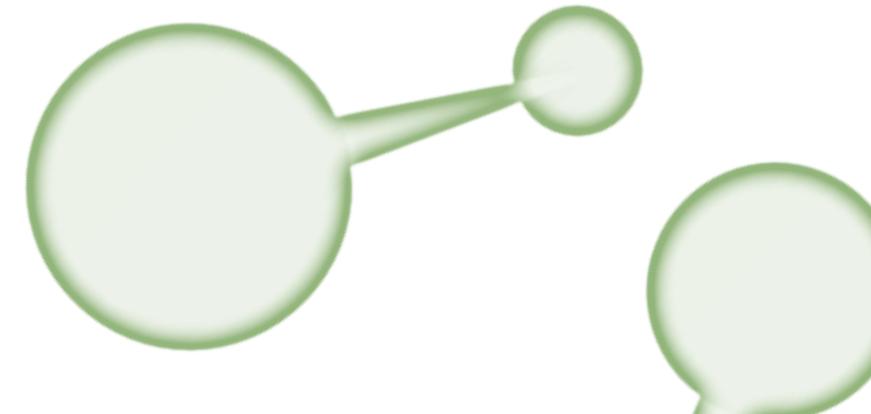
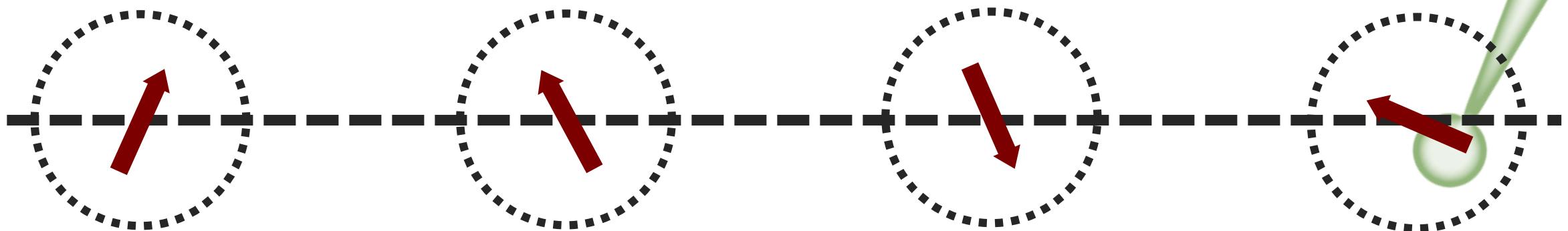


Confinement



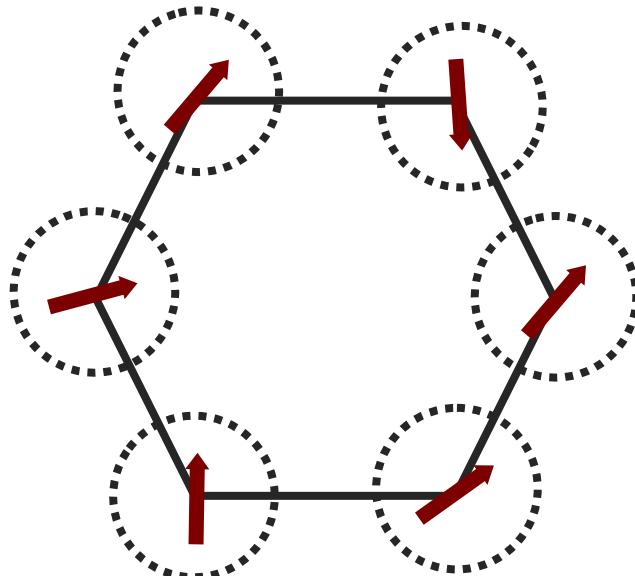
1D Structures

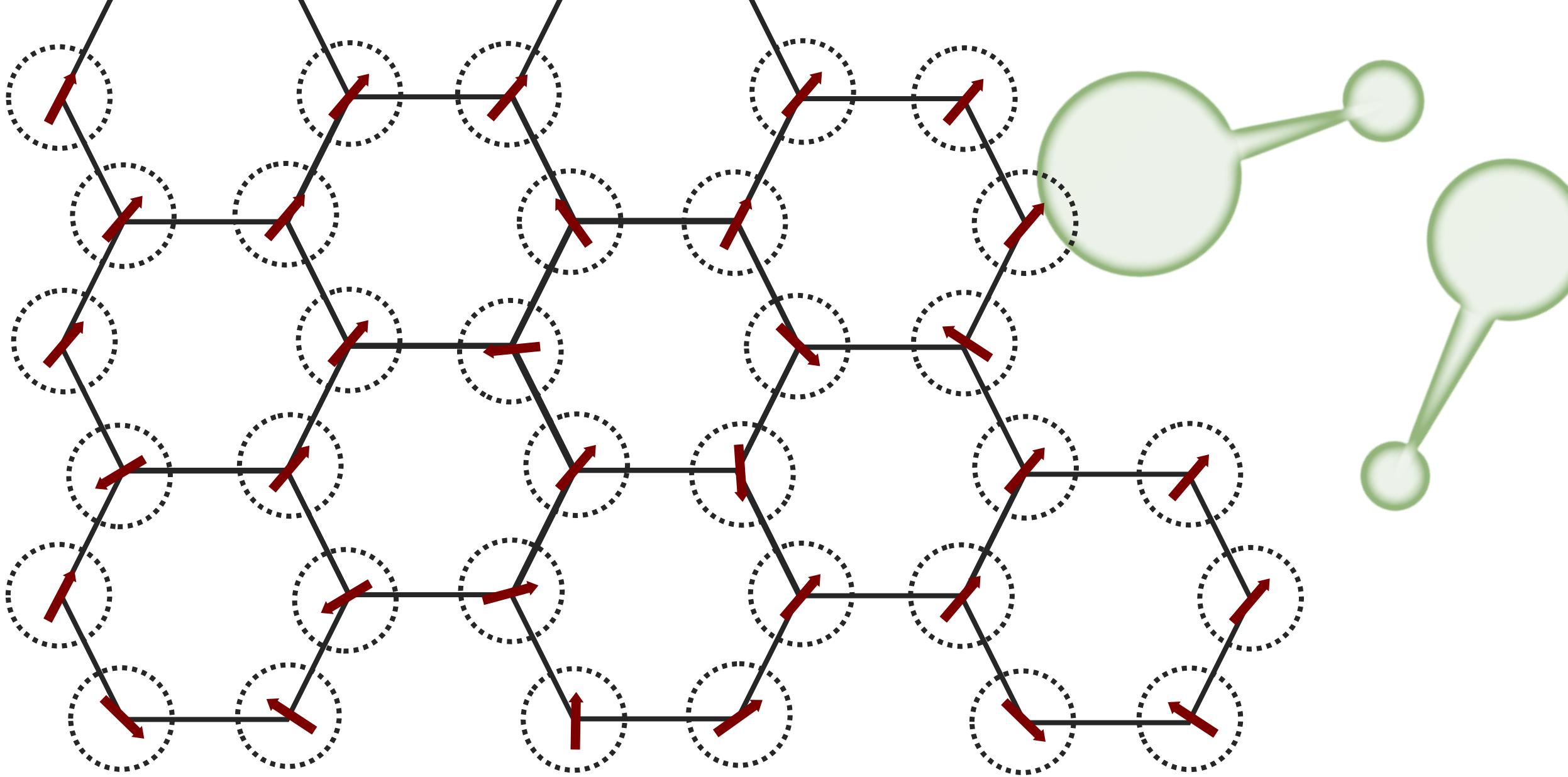
Chains



2D Structures

Lattices





Conclusions

Confined Water

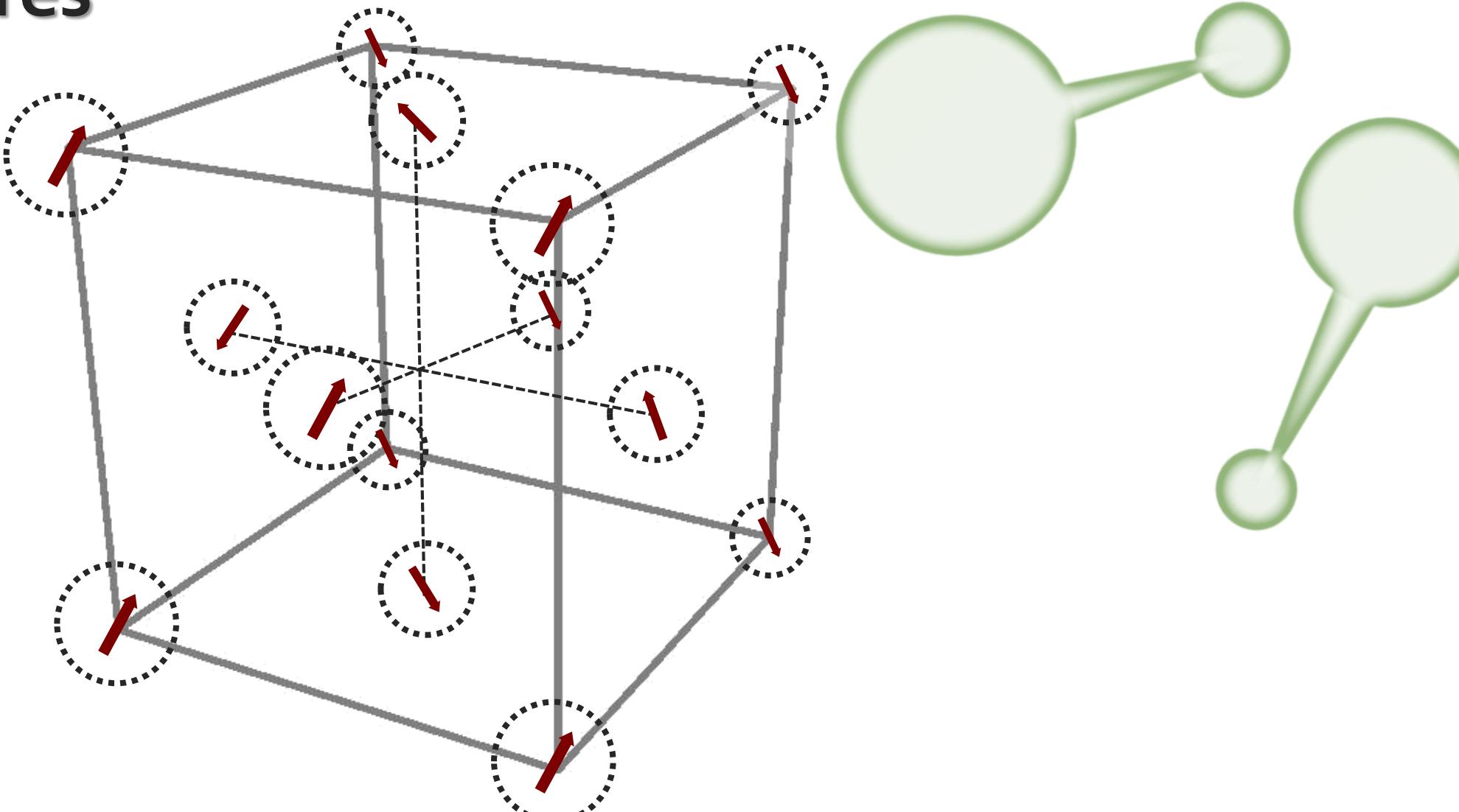
Dipole Chains

Hydrogen Clusters

Overview

3D Structures

Crystals



Conclusions

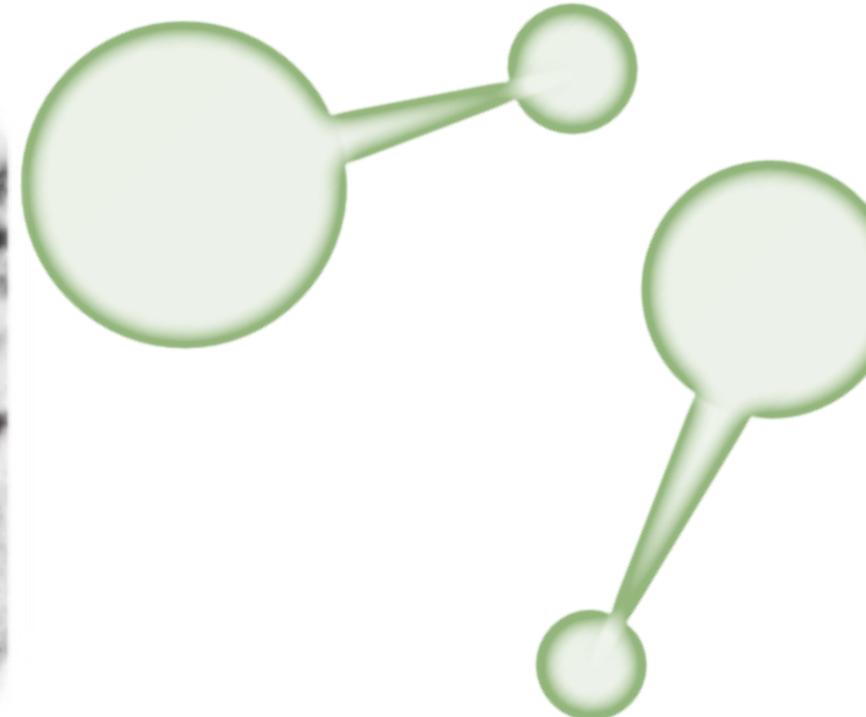
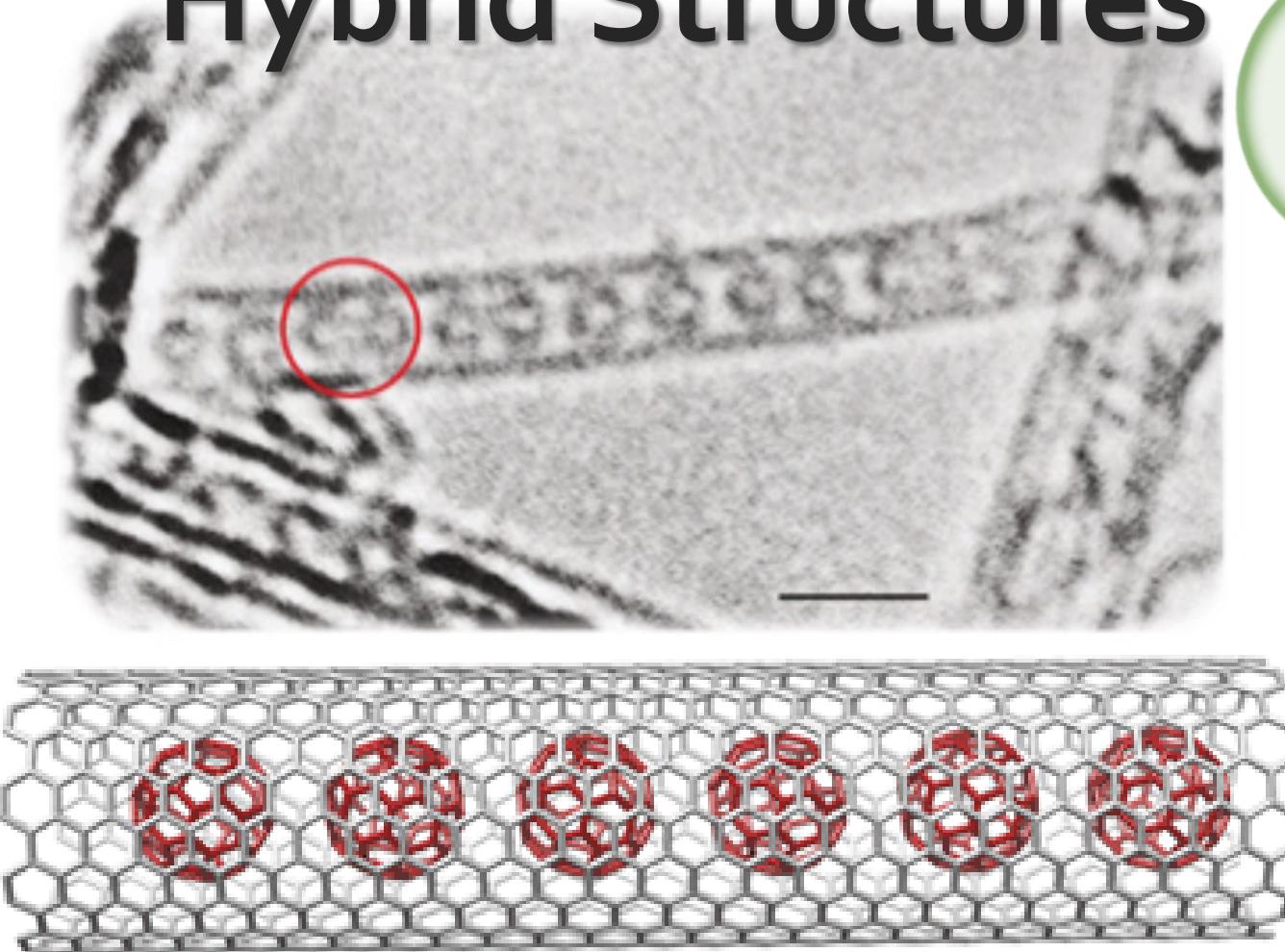
Confined Water

Dipole Chains

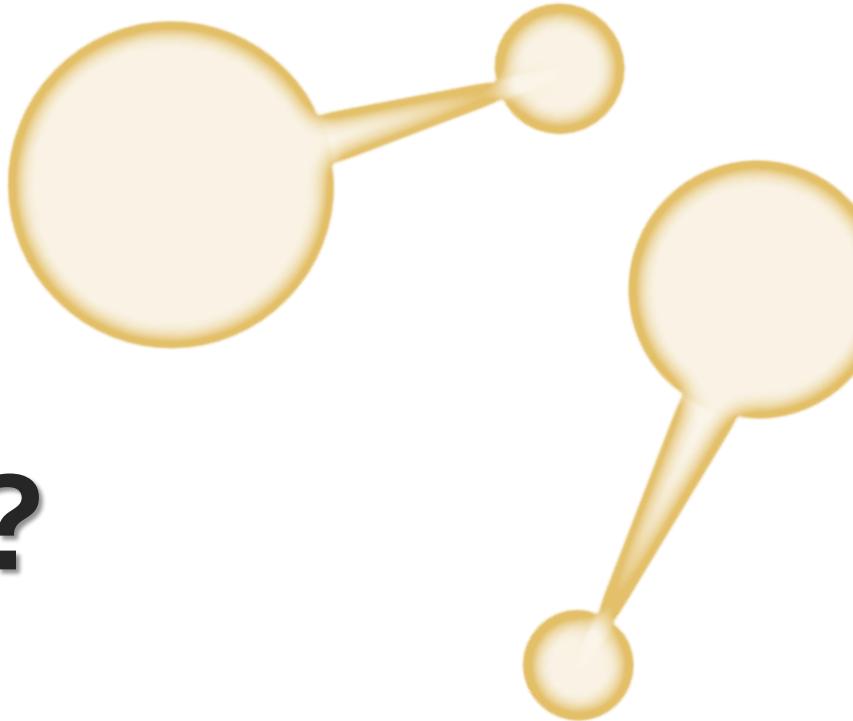
Hydrogen Clusters

Overview

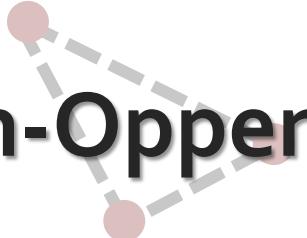
Hybrid Structures



A. de Huan and E. M. Perez, *Nanoscale* 5, 7141 (2013)

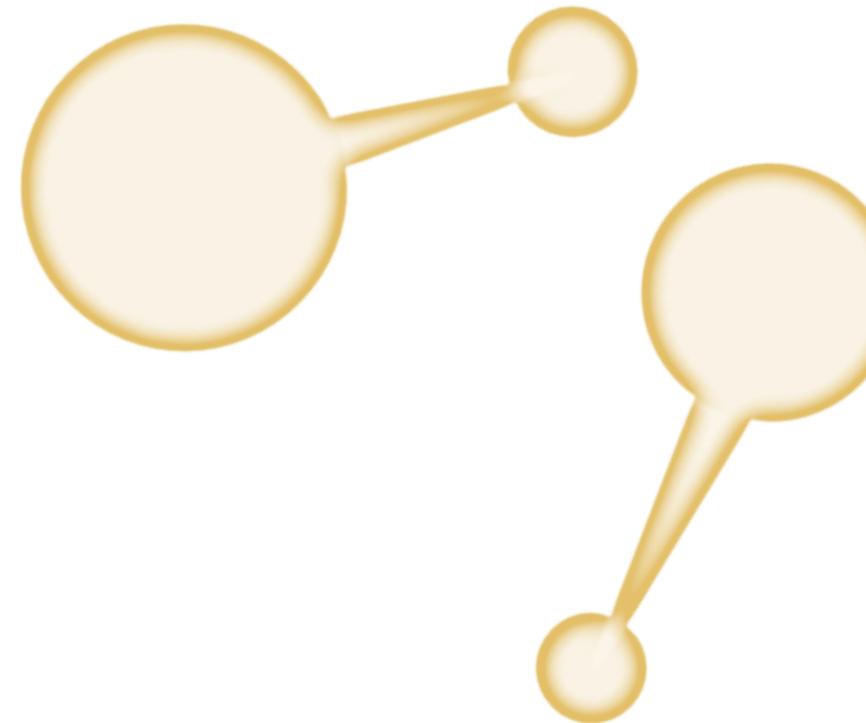


What did we learn?



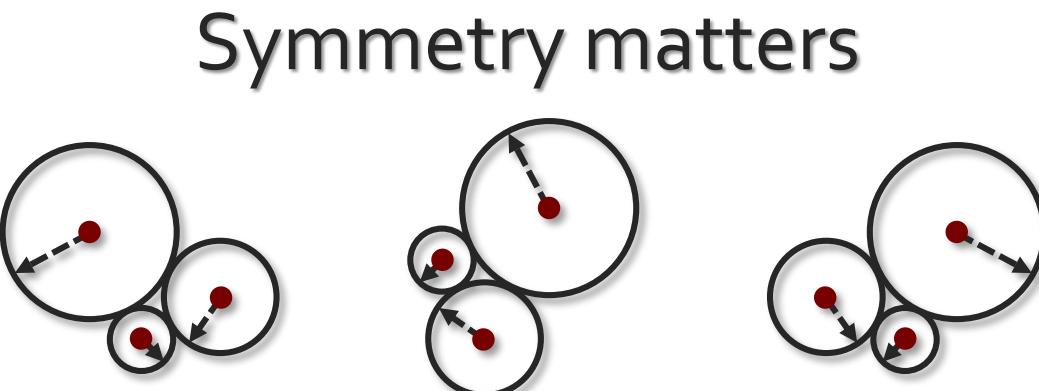
Born-Oppenheimer-Like

Think: Electronic Structure

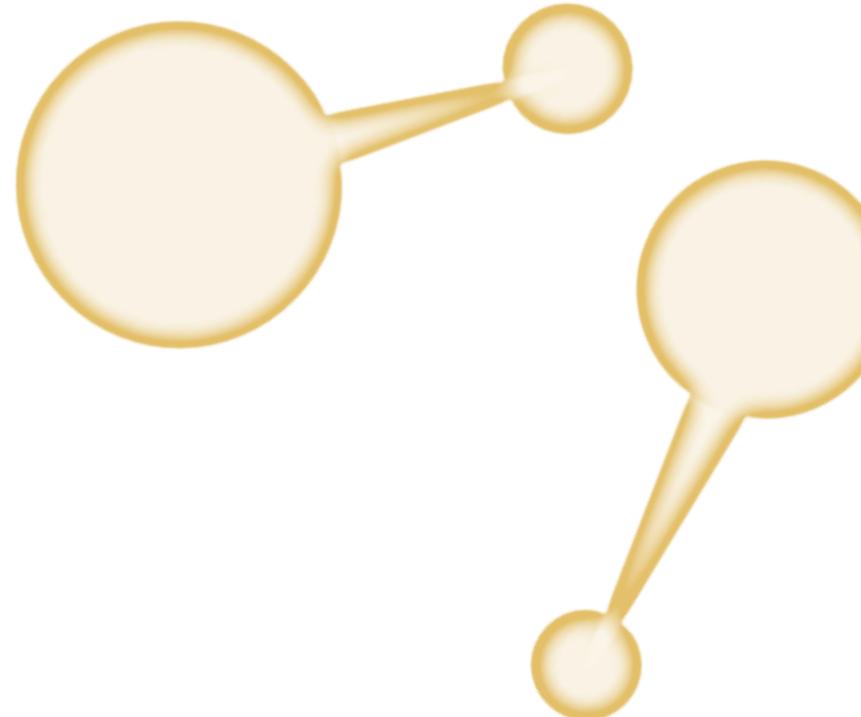


Born-Oppenheimer-Like

Think: Electronic Structure



Symmetry matters

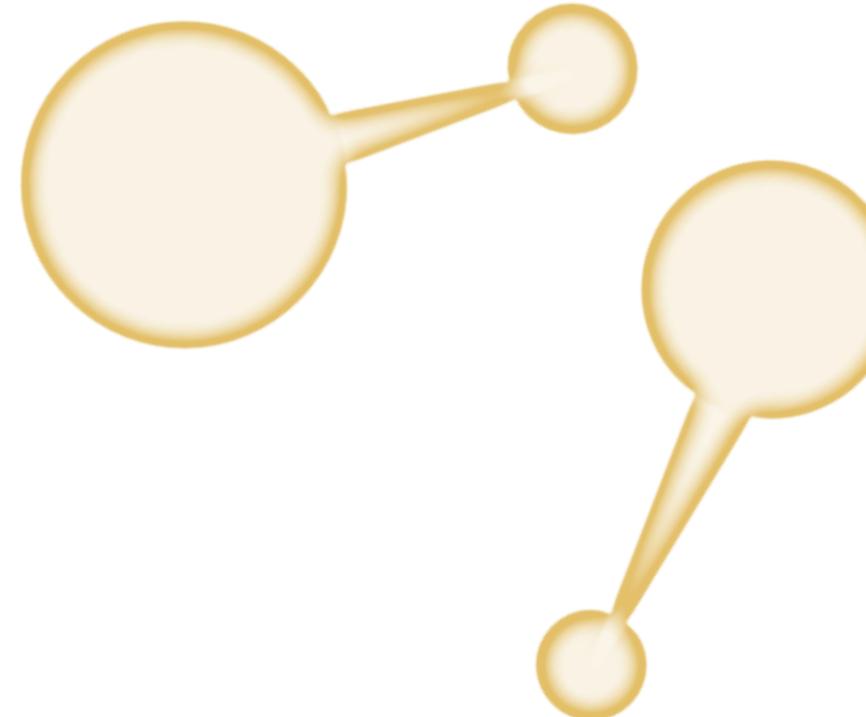
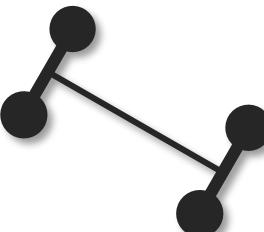
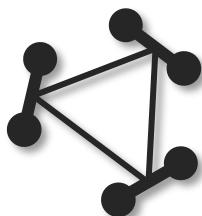


Born-Oppenheimer-Like

Think: Electronic Structure



Many Body effects are significant



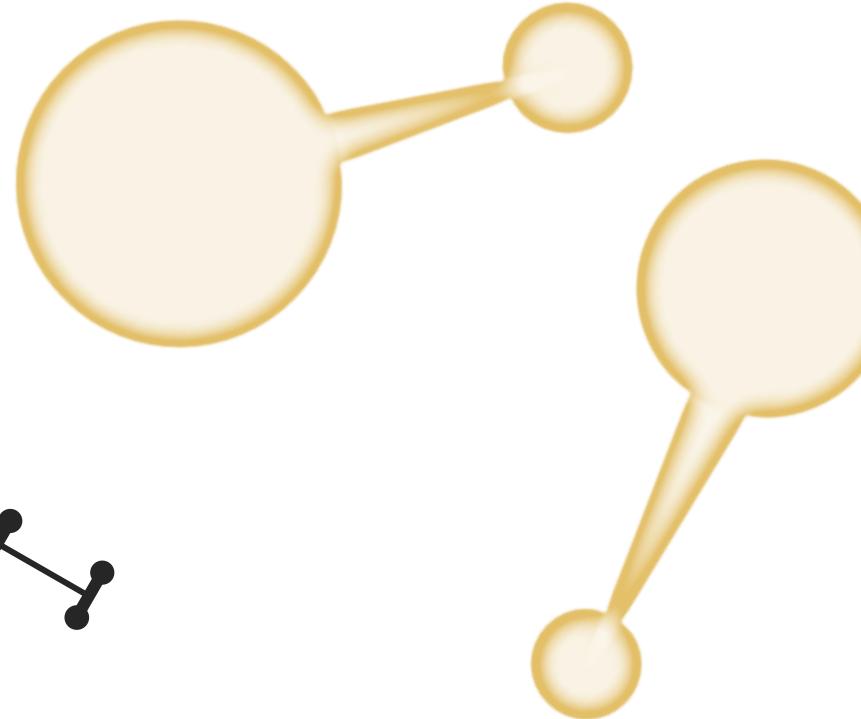
Born-Oppenheimer-Like

Think: Electronic Structure

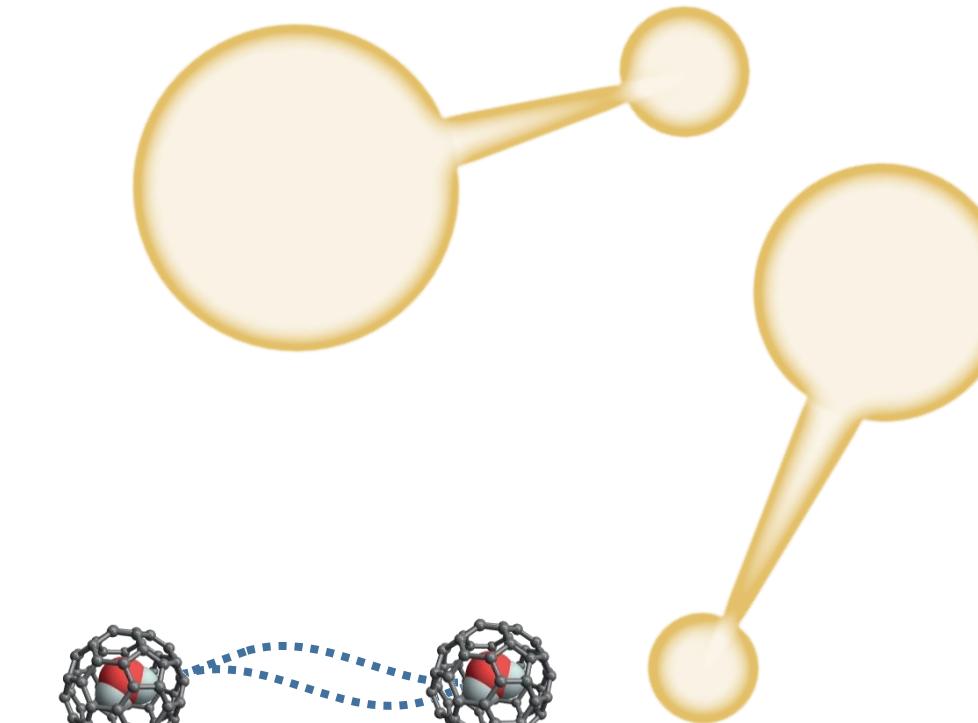
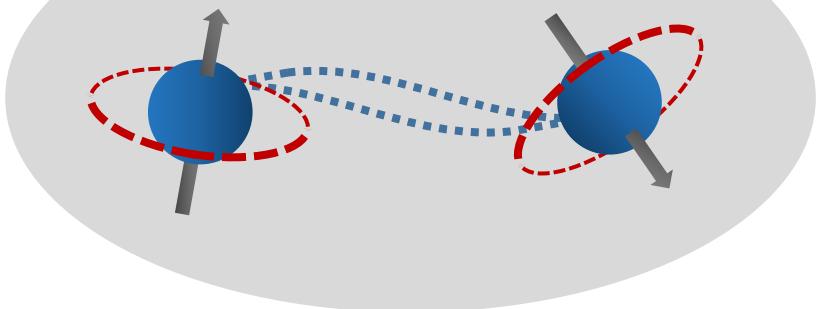


Many Body effects are significant

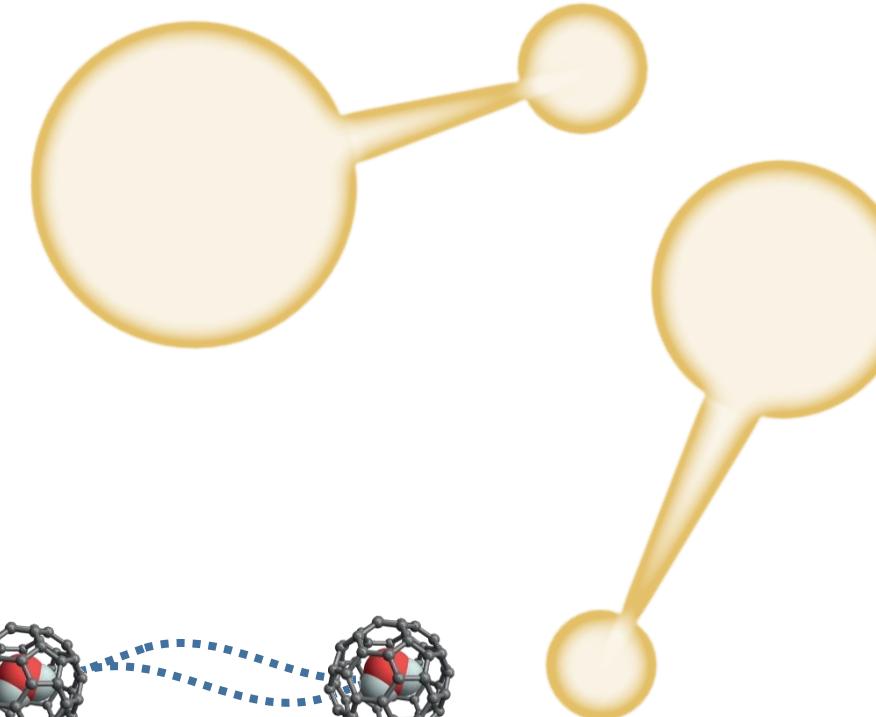
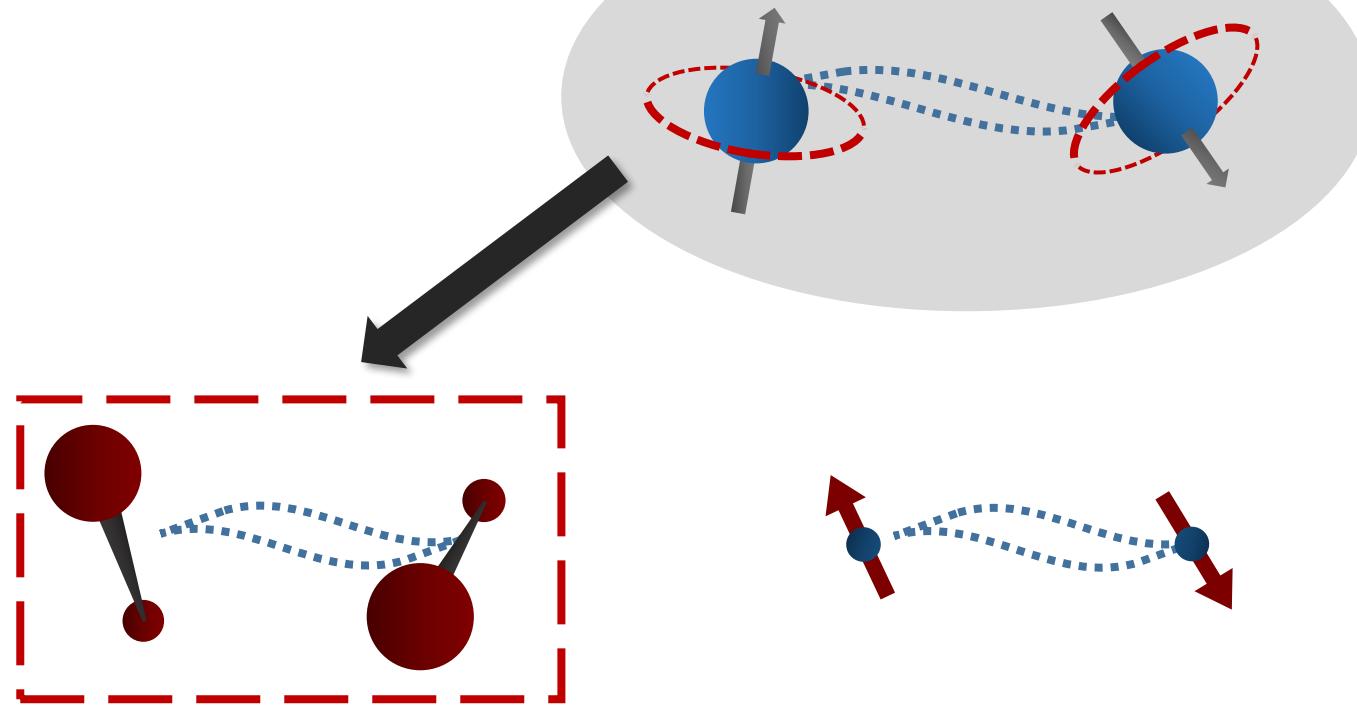
Can we go bigger?



Entanglement

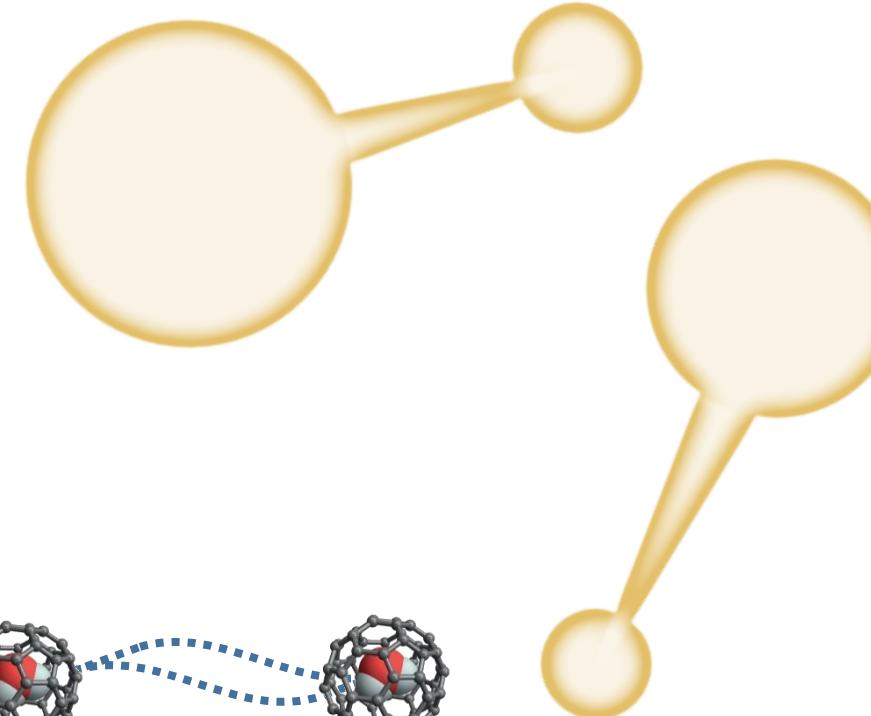
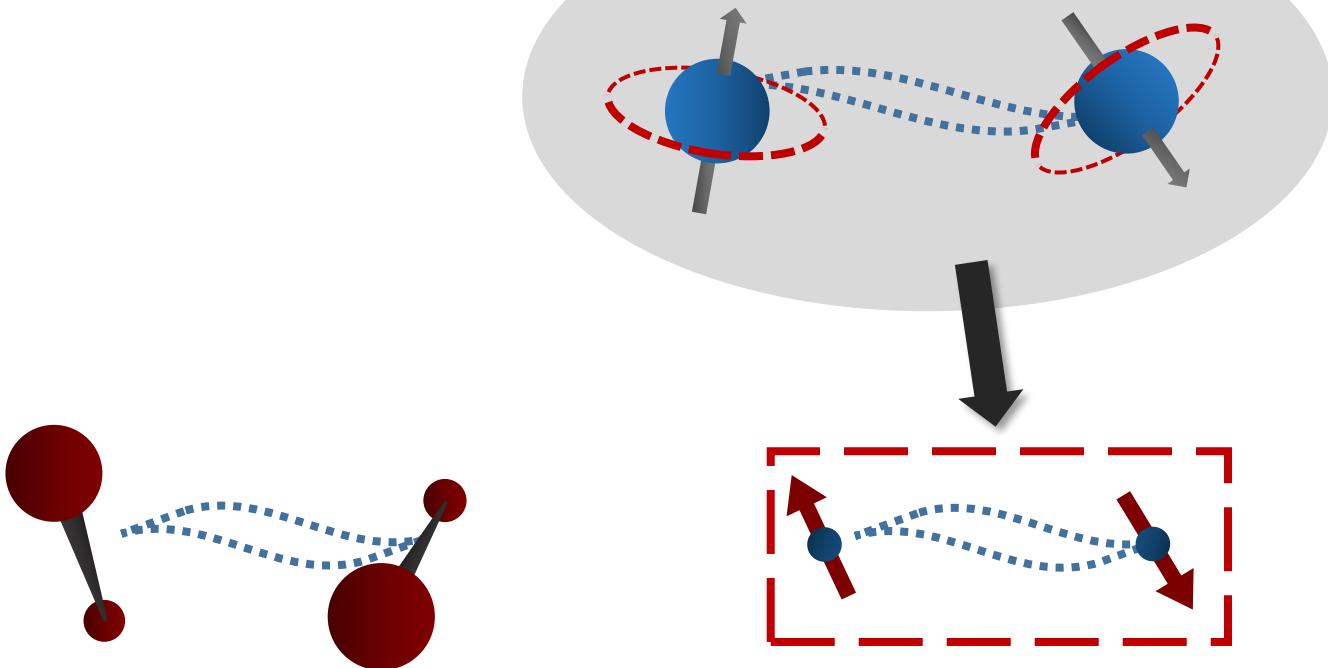


Entanglement



Interaction too weak

Entanglement

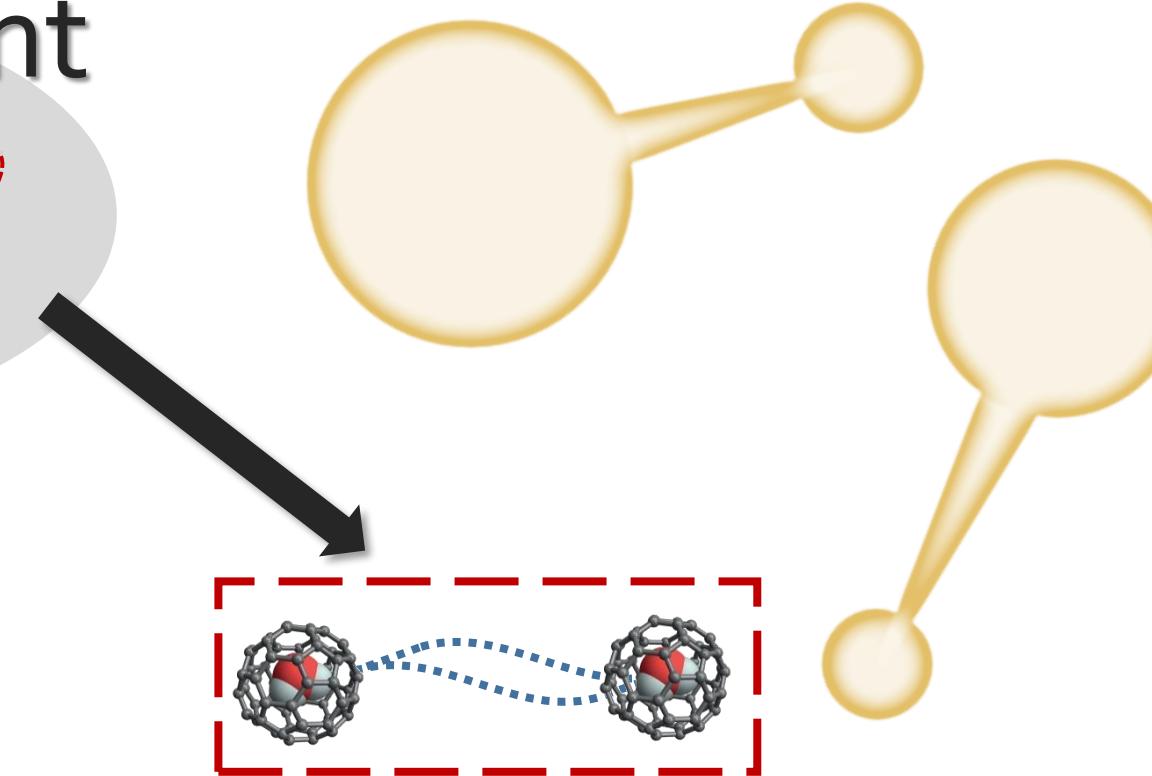
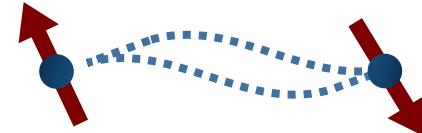
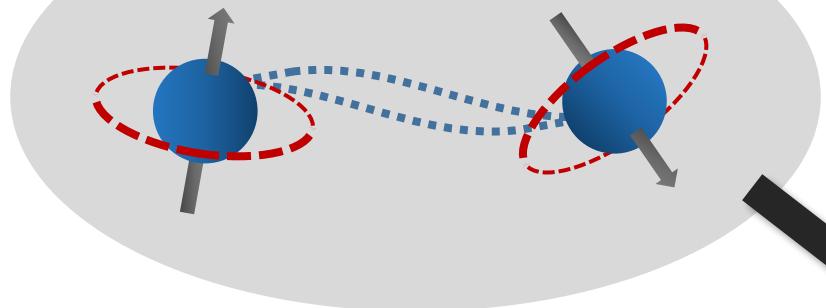


Physically unrealistic

Entanglement



The future?



QAMTS 2017

Special Thanks

Juergen Eckert, Robert McMahon & Amnon Kohen
Bill Poirier & PN Roy



Roy Group

Quantum Molecular Dynamics
Computational and Theoretical Chemistry



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