Three-body Recombination Between Helium and Silver Atoms at Cold Collision Energies

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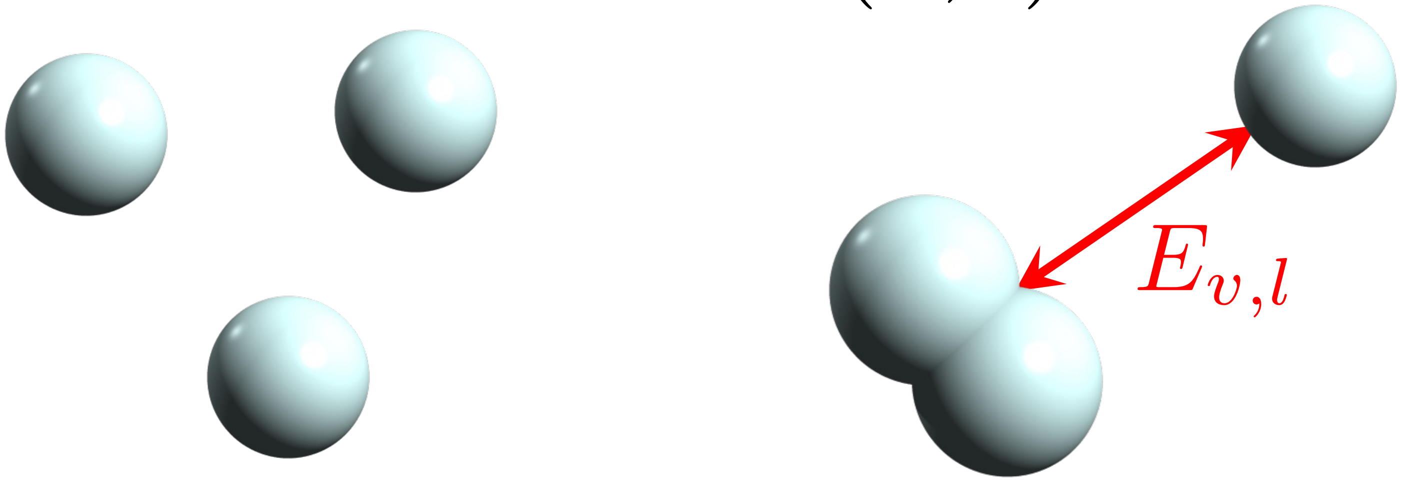
25th European Conference on Few-Body Problem in Physics

1st August 2023, Mainz Germany

Three-Body Recombination

$$\mathrm{A} + \mathrm{A} + \mathrm{A} \rightarrow \mathrm{A}_2(v, l) + \mathrm{A} + E_{v,l}$$



- Two combine into a molecule, the 3rd one dissipates the energy.
- Fundamental & ubiquitous chemical reaction
- Relevant to a wide variety of systems from Astro- to ultracold physics
- Important especially in buffer-gas cooling experiments

The Scope of This Work: 3B Recomb. Between He and Ag

$$\mathrm{He} + \mathrm{He} + \mathrm{Ag} \quad \rightarrow \quad \mathrm{He}_2(0,0) + \mathrm{Ag} + E^{\mathrm{HeHe}}_{0,0}$$

$$\rightarrow \quad \mathrm{HeAg}(v,l) + \mathrm{He} + E^{\mathrm{HeAg}}_{v,l}$$

- Relevant to buffer-gas-cooling experiments by Brahms et al.

PRL **105,** 033001 (2010) PHYSICAL REVIEW LETTERS week ending 16 JULY 2010

Formation of van der Waals Molecules in Buffer-Gas-Cooled Magnetic Traps

N. Brahms,[1,2] T. V. Tscherbul,[2,3] P. Zhang,[3] J. Kłos,[4] H. R. Sadeghpour,[3] A. Dalgarno,[2,3] J. M. Doyle,[2,5] and T. G. Walker[6]

		X^3He		X^4He	
Atom	State	$-\epsilon_0$ [a]	$\frac{n_{X\mathrm{He}}}{n_X}$ [b]	$-\epsilon_0$ [a]	$\frac{n_{X\mathrm{He}}}{n_X}$ [b]
N	$^4S_{3/2}$	2.13	8.3	2.85	0.017
P	$^4S_{3/2}$	2.70	91	3.42	0.046
Cu	$^2S_{1/2}$	0.90	0.015	1.26	5×10^{-4}
Ag	$^2S_{1/2}$	1.40	0.16	1.85	0.0016
Au	$^2S_{1/2}$	4.91	3×10^6	5.87	6.14

- $\mathrm{Ag}^3\mathrm{He}$ and $\mathrm{Ag}^4\mathrm{He}$ v.d.W. molecules observed

Previous Work on 3B Physics

He+He+He→He_2+He

PHYSICAL REVIEW A, VOLUME 65, 042725

Three-body recombination of cold helium atoms

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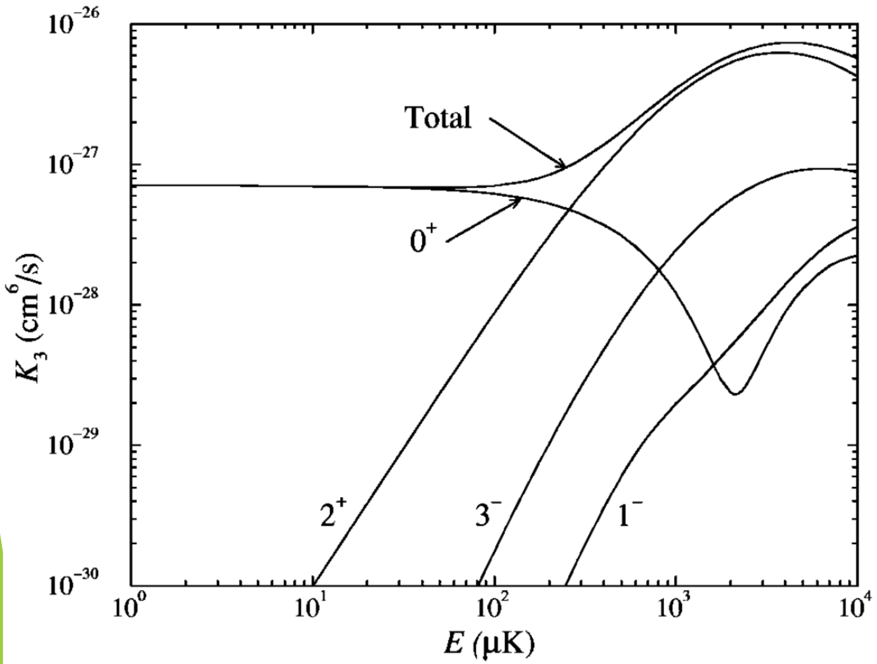
(Received 30 October 2001; published 8 April 2002)



F+F+F→F_2+F

VOLUME 90, NUMBER 5 PHYSICAL REVIEW LETTERS week ending 7 FEBRUARY 2003

Recombination of Three Ultracold Fermionic Atoms

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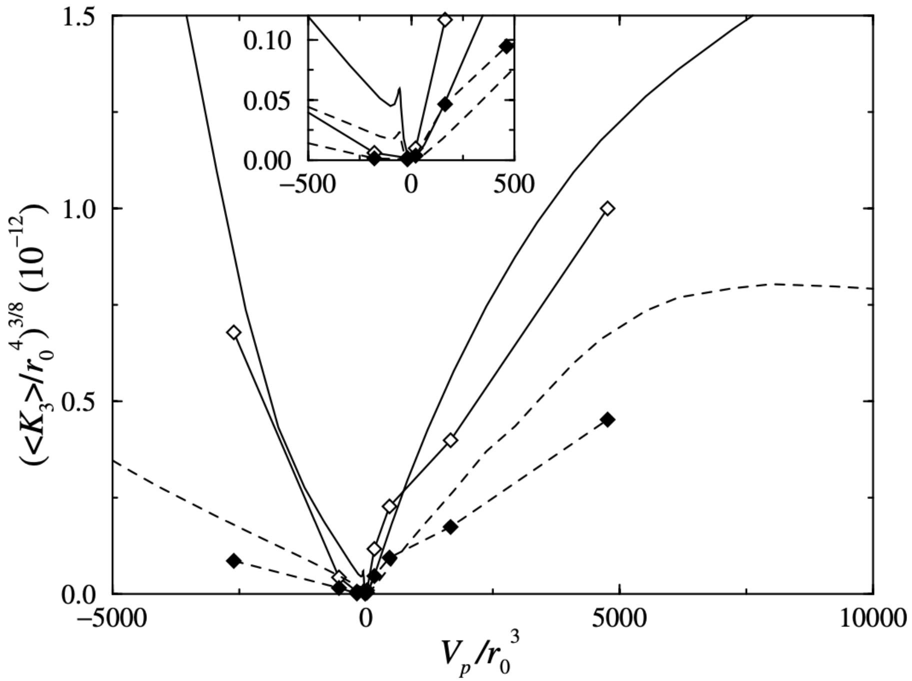
(Received 29 August 2002; published 5 February 2003)

Fermions' Scaling Law: $K_3 \propto |V_p|^{8/3}$



Previous Work on 3B Physics

^{4}He+^{4}He+Alkali→…

PHYSICAL REVIEW A **80**, 062702 (2009)

Three-body recombination in cold helium–helium–alkali-metal-atom collisions

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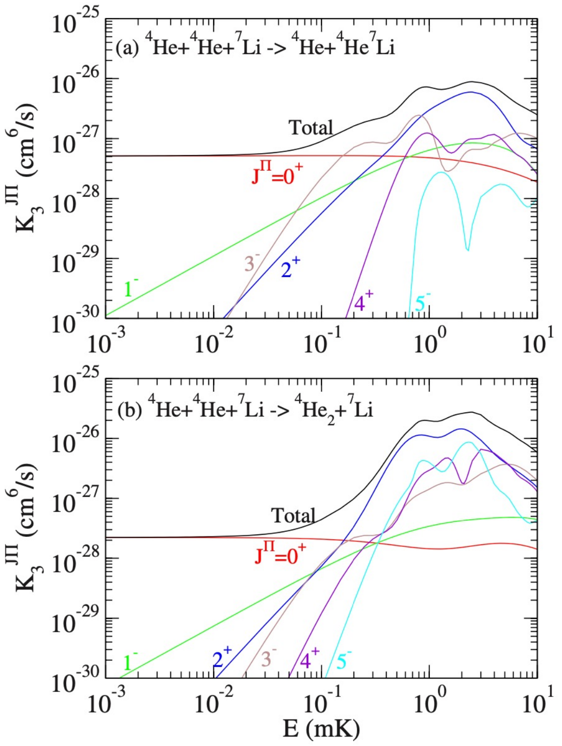

Triple-α Reaction

PHYSICAL REVIEW C **94**, 054607 (2016)

Precise calculation of the triple-α reaction rates using the transmission-free complex absorbing potential method

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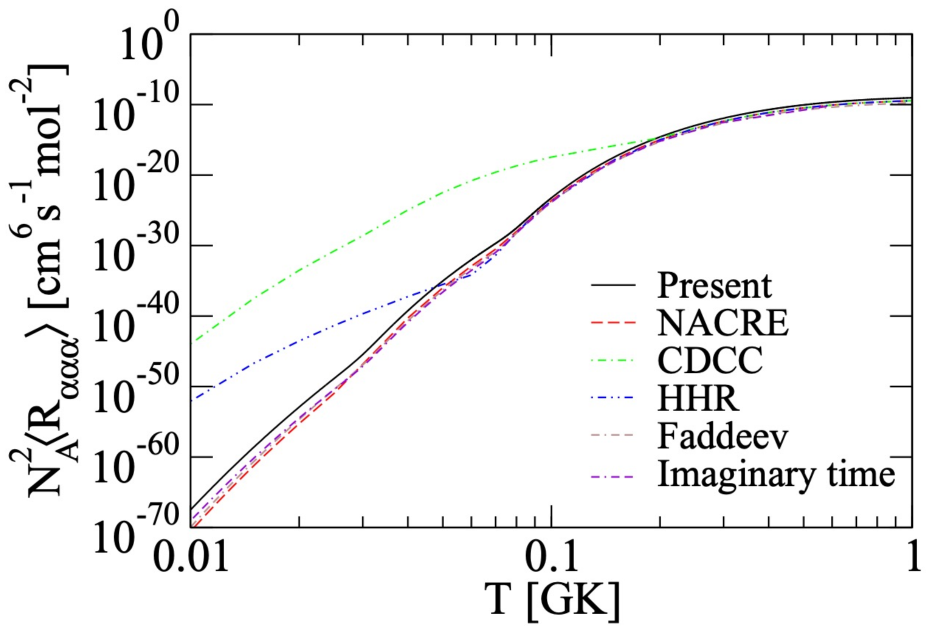


3B Schrödinger Equation in Hyperspherical Coordinates $(R\Omega) \equiv (R\theta\varphi\alpha\beta\gamma)$

$$\left[-\frac{1}{2\mu}\frac{\partial^2}{\partial R^2} + \frac{\Lambda^2 + 15/4}{2\mu R^2} + V(R,\theta,\varphi)\right]\psi_i(R,\Omega) = E\psi_i(R,\Omega)$$

- Grand Angular Momentum Operator:

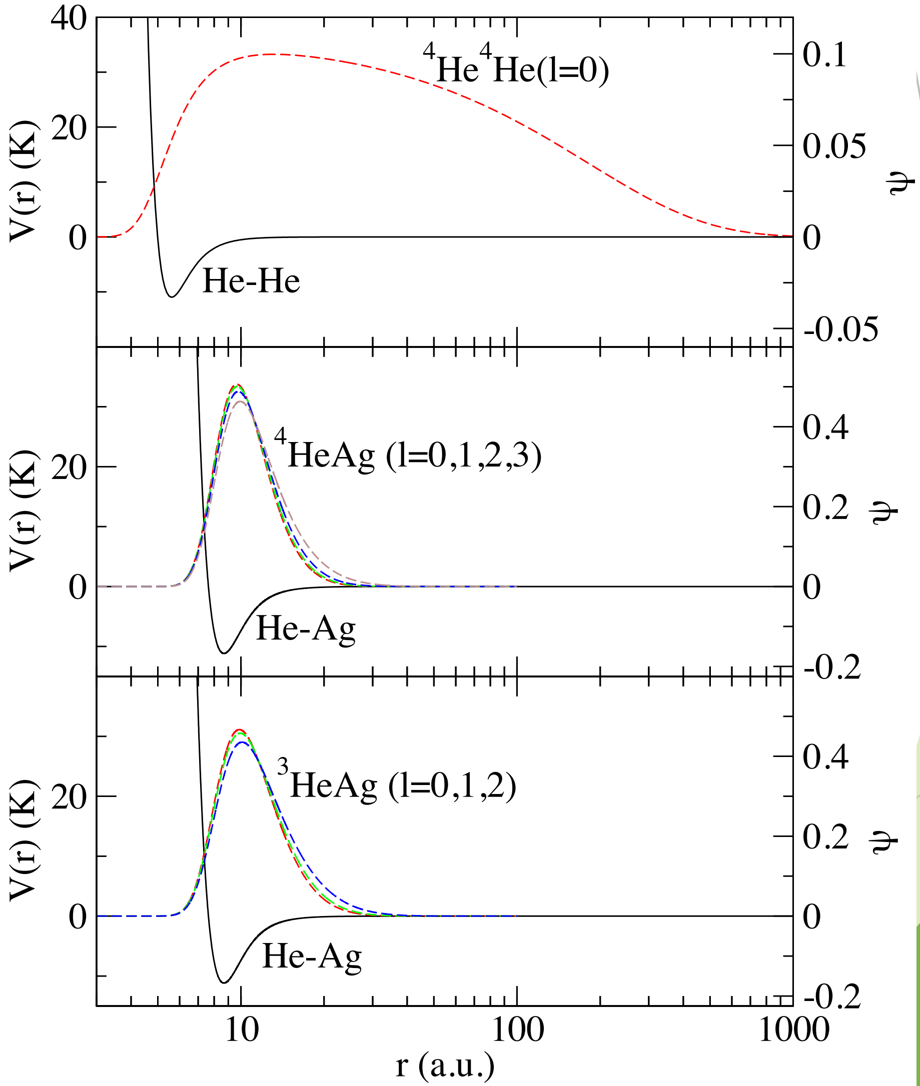
$$\Lambda^2 = -\frac{4}{\sin 2\theta}\frac{\partial}{\partial\theta}\sin 2\theta\frac{\partial}{\partial\theta} + \frac{4}{\sin^2\theta}\left(i\frac{\partial}{\partial\varphi} - \cos\theta\frac{J_z}{2}\right)^2 + \frac{2J_x^2}{1-\sin\theta} + \frac{2J_y^2}{1+\sin\theta} + J_z^2$$

- Body-Fixed Frame Total Angular Momentum: $\mathbf{J} = (J_x J_y J_z)$

Potential-Energy Surface for He_2Ag

$$V(R,\theta,\varphi) = v_{\mathrm{HeAg}}(r_{12}) + v_{\mathrm{HeHe}}(r_{23}) + v_{\mathrm{HeAg}}(r_{31})$$

- He-He Interaction: LM2M2 Rep. by Aziz&Slaman
- $^4He_2$ supports one l=0 bound state.
- He-Ag Interaction: Analytical Form by Xie et al., Data by Gardner et al.
- ^{4}HeAg supports one bound state each with l=0,1,2,3.
- ^{3}HeAg supports one bound state each with l=0,1,2.

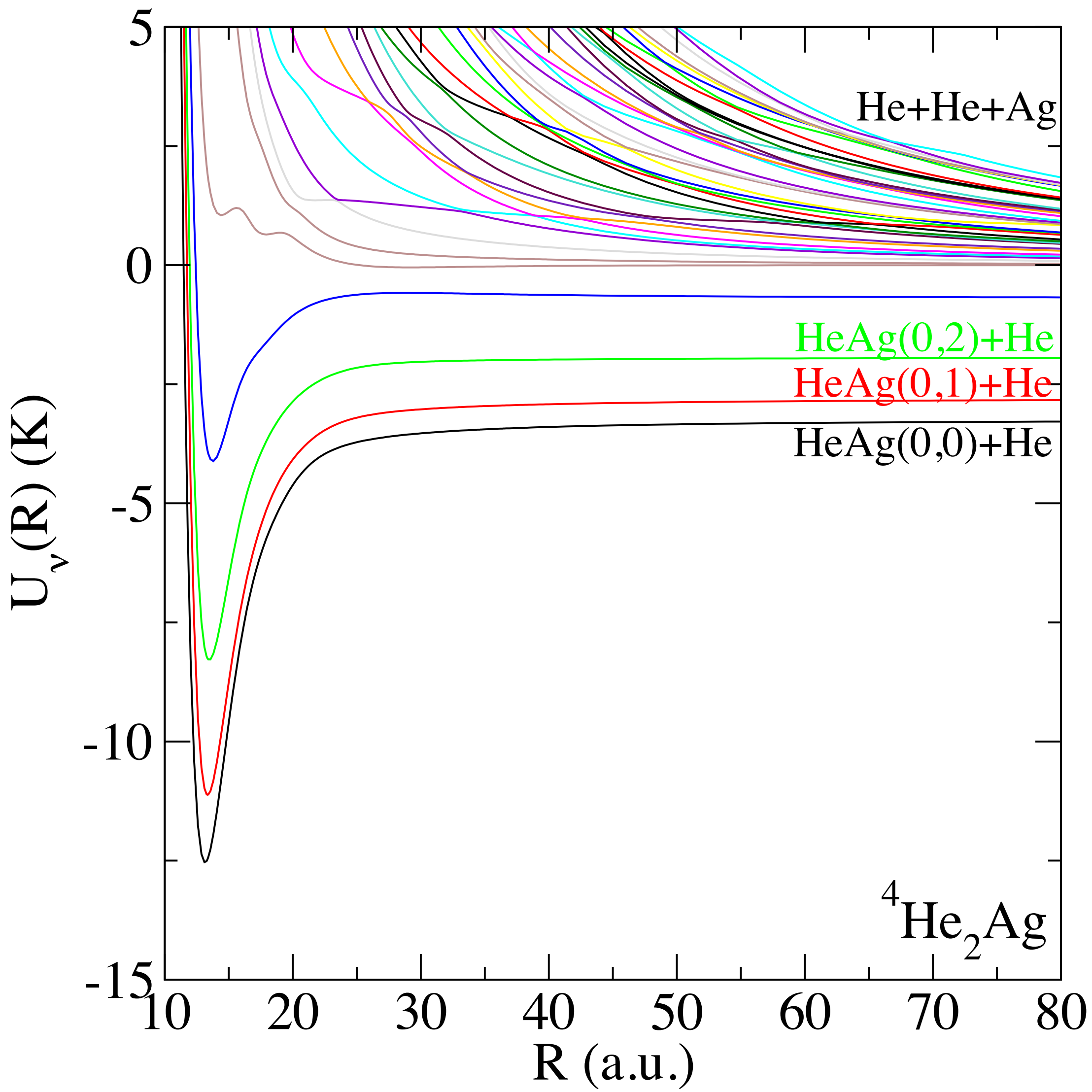


We first solve the fixed-R adiabatic Schrödinger equation: $H_{\mathrm{ad}}(R,\Omega)\Phi_\nu(R;\Omega) = U_\nu(R)\Phi_\nu(R;\Omega)$

- Adiabatic Hamiltonian:

$$H_{\mathrm{ad}}(R,\Omega) = \frac{\Lambda^2}{2\mu R^2} + \frac{15}{8\mu R^2} + V(R,\theta,\varphi)$$

- Potential Curves: $U_\nu(R)$
- Channel Functions: $\Phi_\nu(R;\Omega)$
- Give insight into the structure of the system.



R-matrix Propagation Method

- Propagates, from small to large hyperradii *R*, the R-matrix: $\underline{\mathcal{R}}(R) = \underline{F}(R)[\underline{\tilde{F}}(R)]^{-1}$

$$F_{\nu i}(R) = \int d\Omega \Phi_\nu(R;\Omega)^* \psi_i(R,\Omega),\ \tilde{F}_{\nu i}(R) = \int d\Omega \Phi_\nu(R;\Omega)^* \frac{\partial}{\partial R}\psi_i(R,\Omega)$$

- The hyperradial range is divided up into many subranges, across each of which the R-matrix is propagated. The propagation from a_1 to a_2 is given by

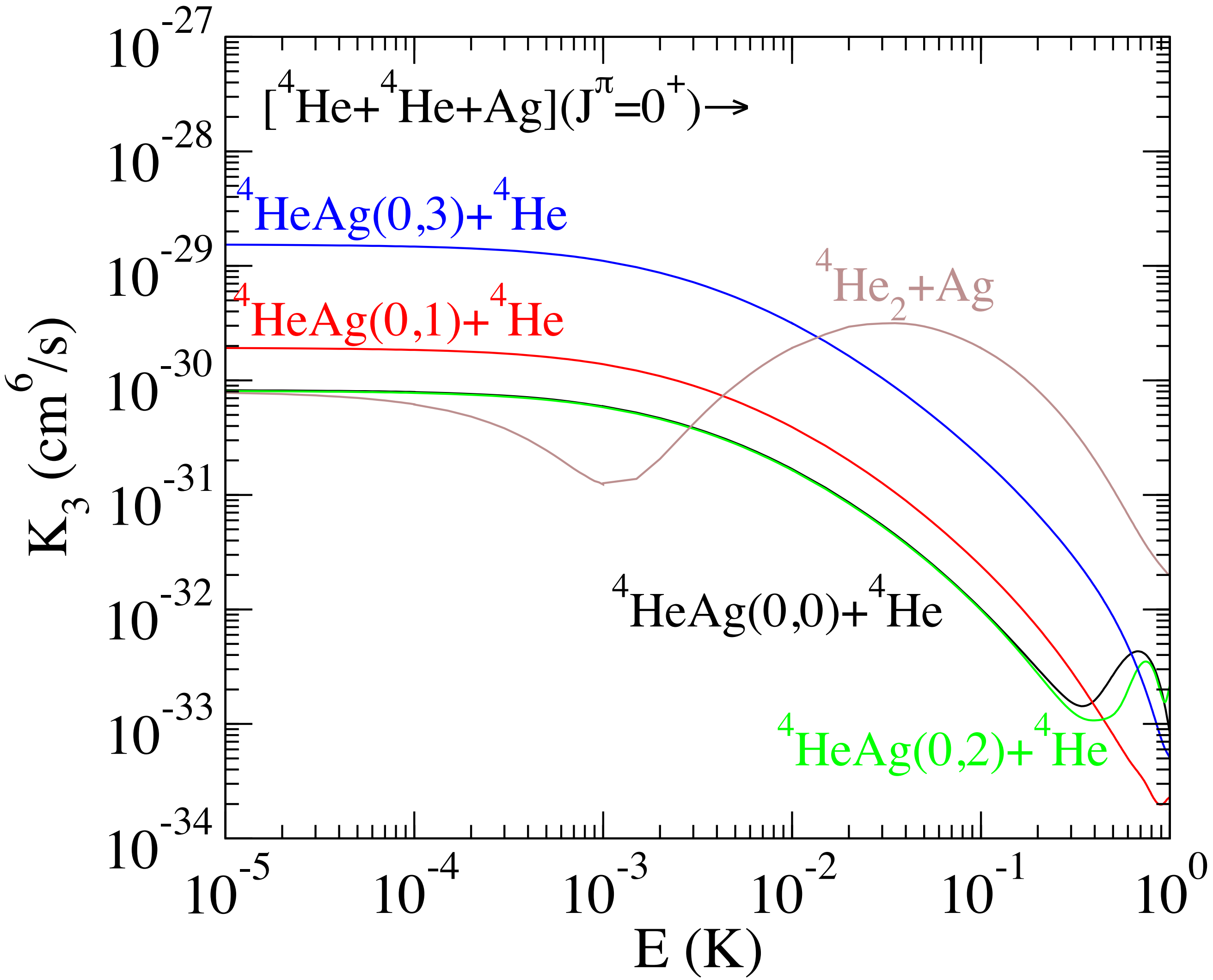
$$\underline{\mathcal{R}}(a_2) = \underline{\mathcal{R}}_{22} - \underline{\mathcal{R}}_{21}[\underline{\mathcal{R}}_{11} + \underline{\mathcal{R}}(a_1)]^{-1}\underline{\mathcal{R}}_{12}$$

- The coefficient matrix R11, R12, R21, R22 are calculated by solving the Schrödinger equation within the subrange $[a_1, a_2]$:

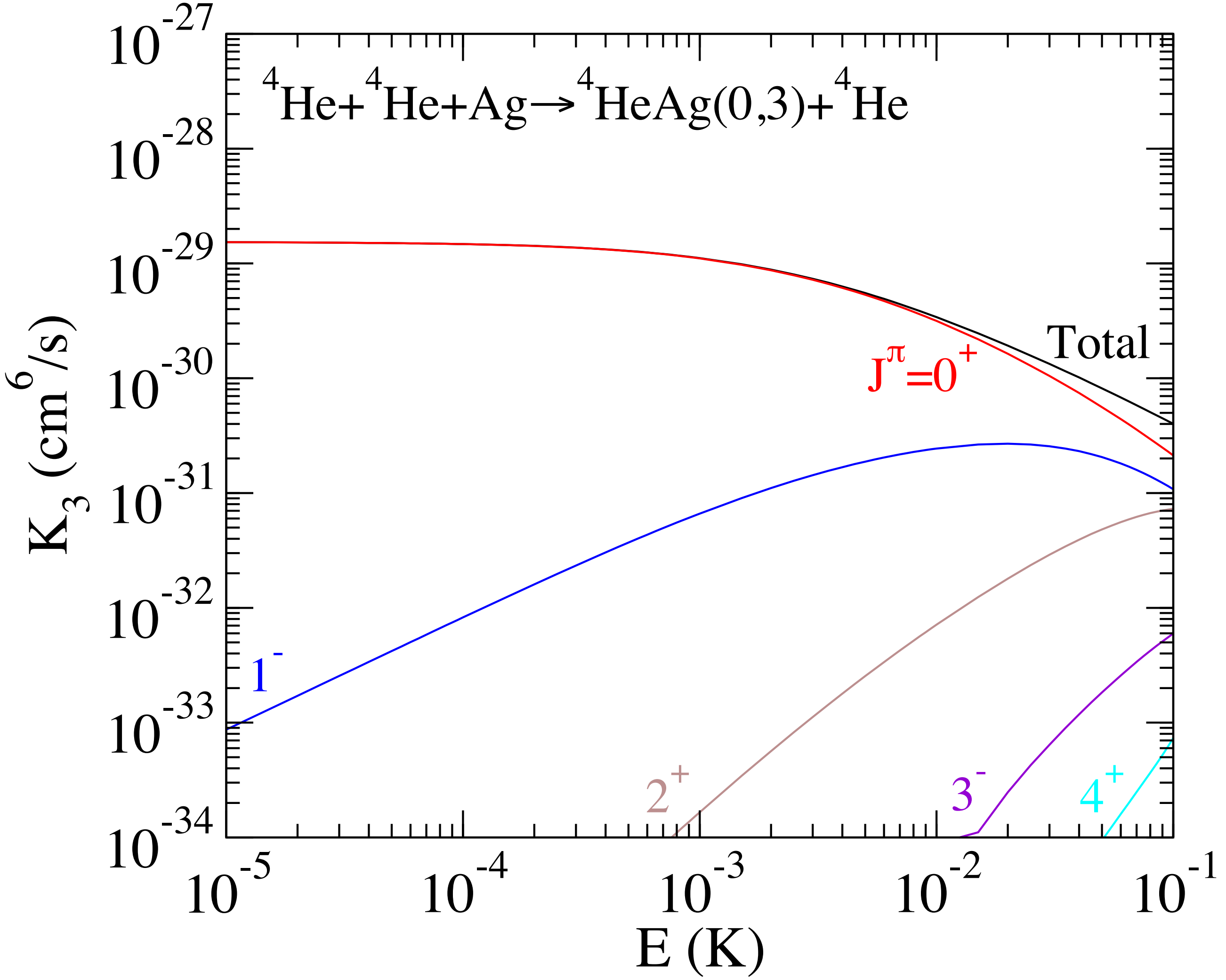
$$\vec{x}_n^T \mathcal{H} \vec{x}_{n'} = \varepsilon_n \delta_{nn'}$$

- H is the Discrete Variable Representation (DVR) Hamiltonian matrix given either by the Smooth Variable Discretization approach (small R) or by the adiabatic approach (large R).
- Three-body recombination rate: $K_3 = \sum_{J,\pi,\kappa} \sum_{i,f} \frac{192\pi^2(2J+1)}{\mu k^4} |\mathcal{S}_{fi}^{J\pi\kappa}|^2$
- For details, see J.Wang et al. PRA2011.

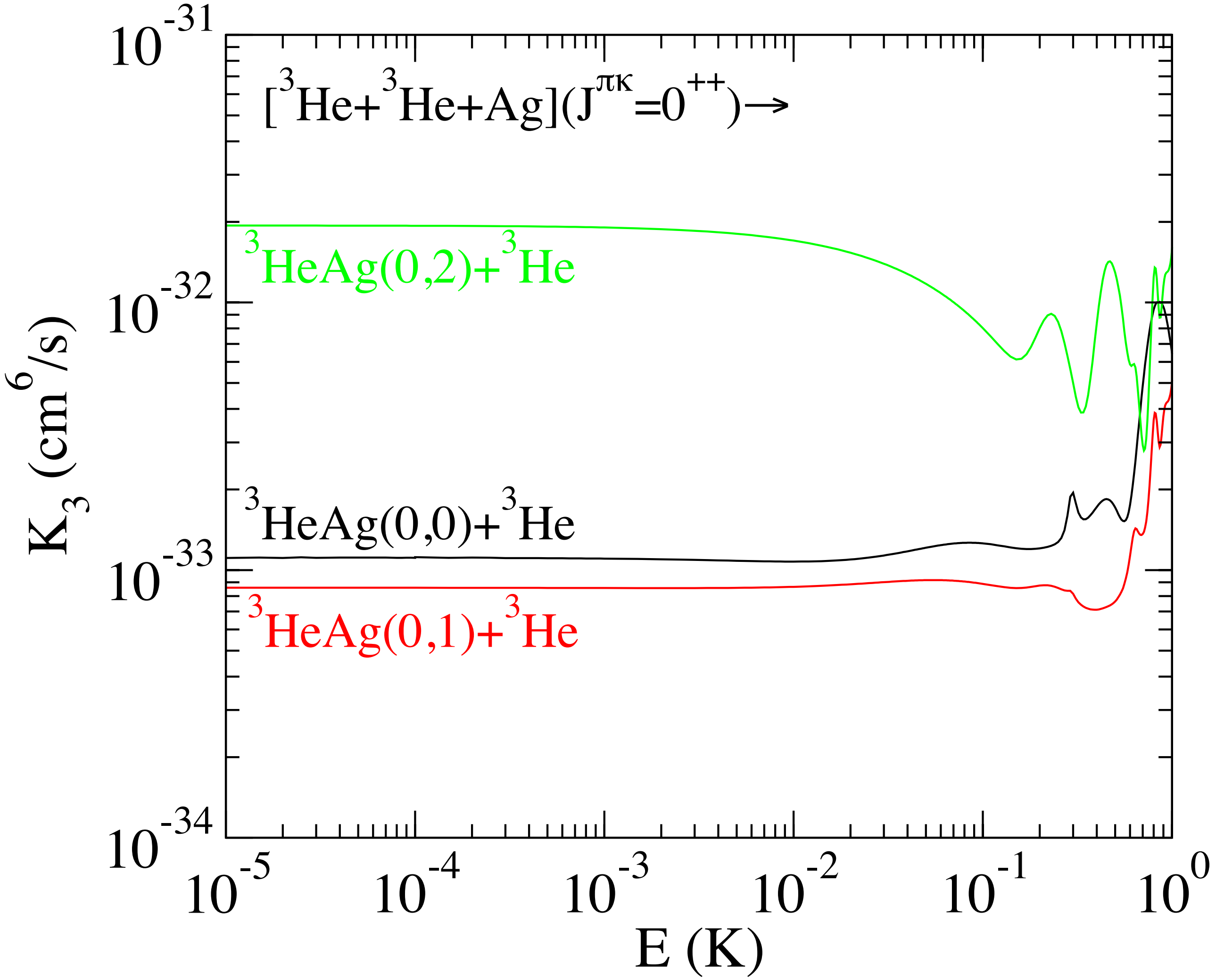
$J^\pi = 0^+$ Partial 3B Recombination Rates for $^4He+^4He+Ag$



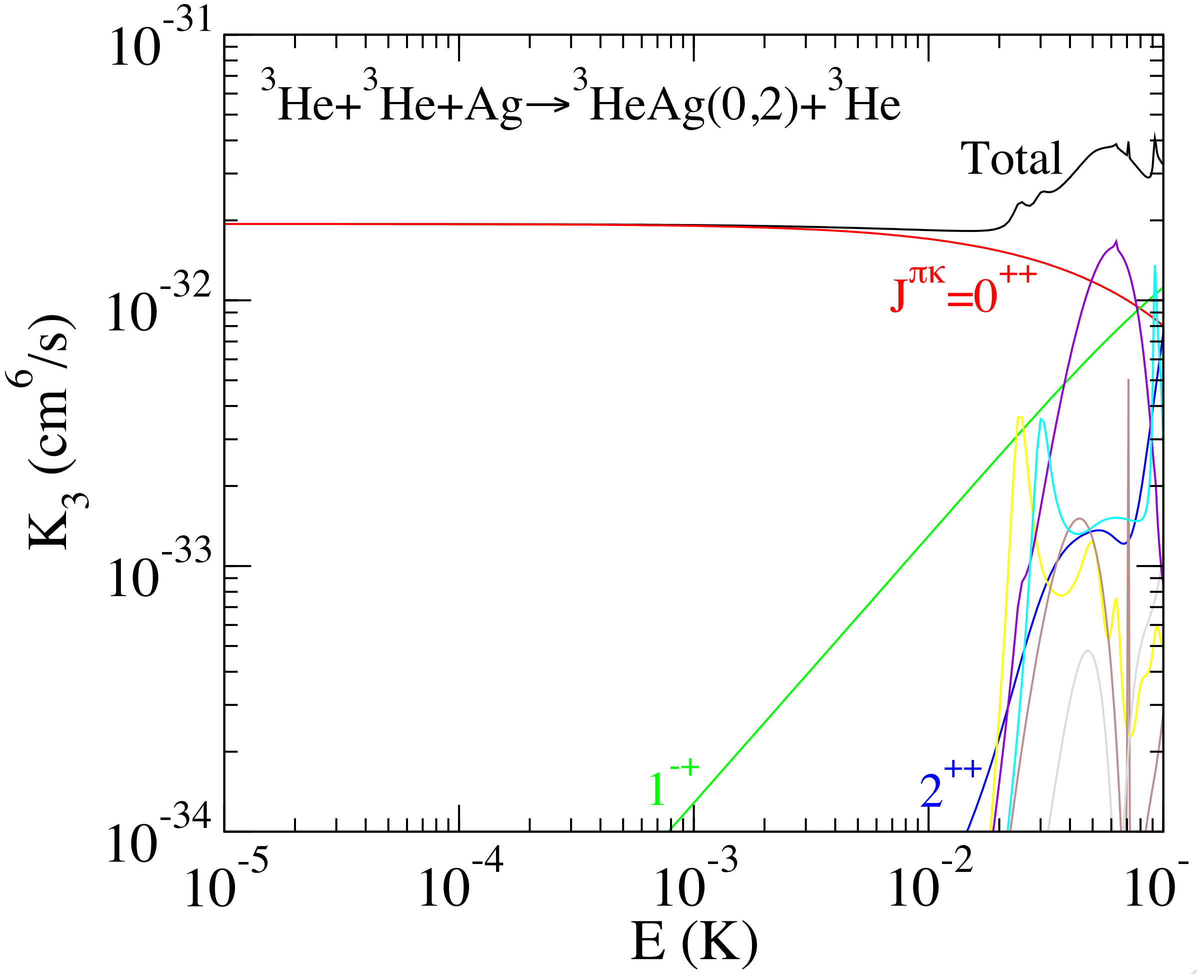
$J \geq 0$ Recombination Rates for $^4He+^4He+Ag\rightarrow{}^4HeAg(v=0,l=3)+^4He$



$J^{\pi\kappa} = 0^{++}$ Partial 3B Recombination Rates for ^3He+^3He+Ag



$J \geq 0$ Recombination Rates for $^3He + ^3He + Ag \rightarrow ^3HeAg(v=0, l=2) + ^3He$



At >10^-2, got complicated, need to be checked!

Summary

- Considered the 3B recombination processes He+He+Ag->HeAg+He,He_2+Ag
- The Schrödinger Eq. represented by the SVD and the adiabatic approaches is solved.
- The three-body recombination rates for ^{4}He+^{4}He+Ag at threshold are found to be generally less than about 10^{-29}, one or two order smaller than that for ^{4}He+^{4}He+^{4}He, ~10^{-27}.
- The recombination rates for ^{3}He+^{3}He+Ag at threshold are still smaller.
- At higher collision energies, the J>0 rates may contribute in a complicated way, need to be checked.