Few-body systems of positrons and electrons

Adiabatic hyperspherical development

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Outline

- Part I:
  - How to divide and conquer the Hamiltonain
  - “Hyperspherical explicitly correlated Gaussians” or “correlated Gaussian hyperspherical technique”?
  - New matrix element calculation technique
- Part 2:
  - Application to few-body Coulomb systems
  - Outlook

Divide and conquer

Separate off center of mass, focus on relative Hamiltonian (N Jacobi vectors each in d dimensions), and recast in terms of hyperspherical coordinates.

$$H_{\text{rel}} = \mathcal{T} + V_{\text{int}}$$
$$= \mathcal{T}_R + \mathcal{T}_{\mathbf{\Omega}} + V_{\text{int}}(R, \mathbf{\Omega})$$

$$\mathcal{T}_R = -\frac{\hbar^2}{2\mu} \frac{1}{R^{Nd-1}} \frac{\partial}{\partial R} R^{Nd-1} \frac{\partial}{\partial R}$$

Expand solutions in product of radial and so called channel functions. The hyperradius R is our adiabatic parameter.

$$\Psi_E(R, \mathbf{\Omega}) = R^{-(Nd-1)/2} \sum_{\nu} F_{E\nu}(R) \Phi_{\nu}(R; \mathbf{\Omega})$$

Channel functions are orthogonal over the hyperangles (at a fixed R) and solve the adiabatic Hamiltonian.

$$\int d\mathbf{\Omega}\, \Phi_{\nu}^{*}(R; \mathbf{\Omega}) \Phi_{\nu'}(R; \mathbf{\Omega}) = \delta_{\nu\nu'}$$

$$H_{\text{ad}}(R, \mathbf{\Omega}) \Phi_{\nu}(R; \mathbf{\Omega}) = U_{\nu}(R) \Phi_{\nu}(R; \mathbf{\Omega})$$

Divide and conquer

Expansion results in (an infinite number of) coupled 1-D PDE's in R.

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2} + U_\nu(R) - E\right)F_{E\nu}(R) + W = 0$$

coupling

$$W = -\frac{\hbar^2}{2\mu}\sum_{\nu'}\left(2P_{\nu\nu'}\frac{\partial}{\partial R} + Q_{\nu\nu'}\right)F_{E\nu'}(R)$$

Couplings come from imperfect separability in R and Ω; called P and Q matrices.

$$P_{\nu\nu'} = \left\langle \Phi_\nu \middle| \frac{\partial \Phi_{\nu'}}{\partial R} \right\rangle_{\Omega} \qquad Q_{\nu\nu'} = \left\langle \Phi_\nu \middle| \frac{\partial^2 \Phi_{\nu'}}{\partial R^2} \right\rangle_{\Omega}$$

Basis to solve adiabatic Hamiltonian

$$H_{\mathrm{ad}}(R,\mathbf{\Omega}) = \frac{\hbar^2}{2\mu}\frac{(Nd-1)(Nd-3)}{4R^2} + \frac{\hbar^2\Lambda^2}{2\mu R^2} + V_{\mathrm{int}}(R,\mathbf{\Omega})$$

Interactions break separability, so let's choose a basis.
For simplicity, unsymmetrized spherical explicitly correlated Gaussians (ECG).

$$|A\rangle = \prod_{i<j}\exp\left(-\frac{1}{2}\frac{|\boldsymbol{r}_i-\boldsymbol{r}_j|^2}{\alpha_{ij}^2}\right) = \exp\left(-\frac{1}{2}\boldsymbol{x}^T\underline{A}\boldsymbol{x}\right)$$
$$= \exp\left(-\frac{1}{2}R^2 f_A(\mathbf{\Omega})\right)$$

x here is a vector of Jacobi vectors, A the correlation matrix.

Mitroy *et al.*, Rev. Mod. Phys. **85**, 693 (2013)

Matrix element strategy: brute force approach

1. **Switch to coordinates that diagonalize A+A'.**
2. **Integrate over trivial polar angles, e.g. 3-D $\sin(\theta_j)d\theta_j d\phi_j$.**
   Example: overlap integral of two spherical Gaussians

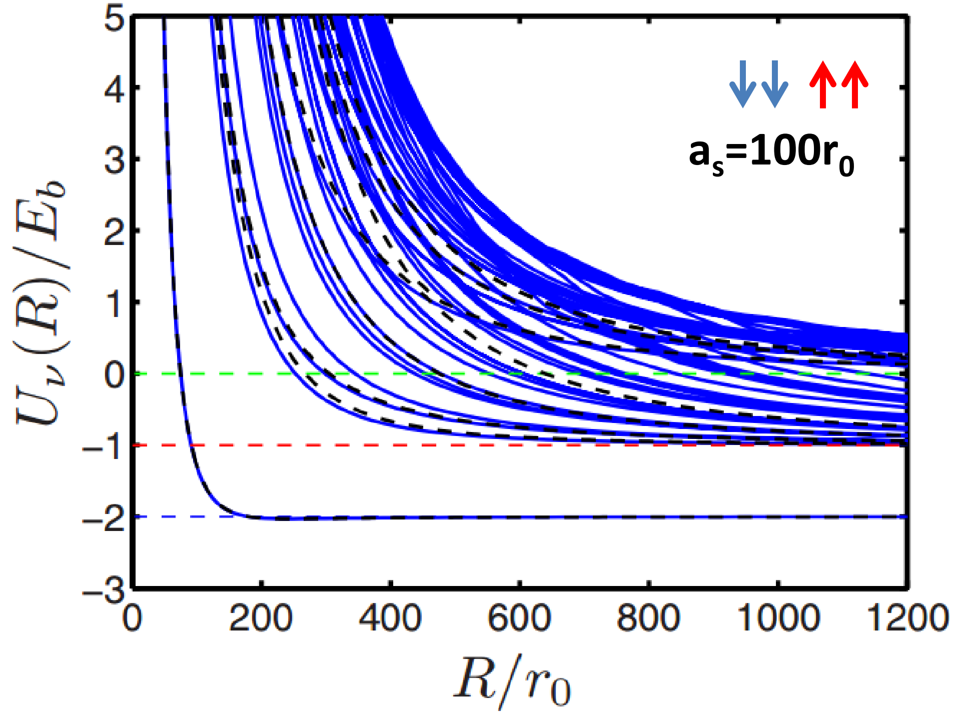
$$\langle A|A'\rangle_{\Omega} = \underbrace{\left[\frac{2\pi^{d/2}}{\Gamma(d/2)}\right]^N}_{\text{Volume element of d-dimensional sphere to N}^{\text{th}}\text{ power}} \int_{N-1} \exp\left(-\frac{R_0^2}{2}[\text{mess of sin's and cos's}]\right) d\bar{\Omega}$$

$$d\bar{\Omega} = (\text{another mess of sin's and cos's}) d\alpha_1 \cdots d\alpha_{N-1}$$

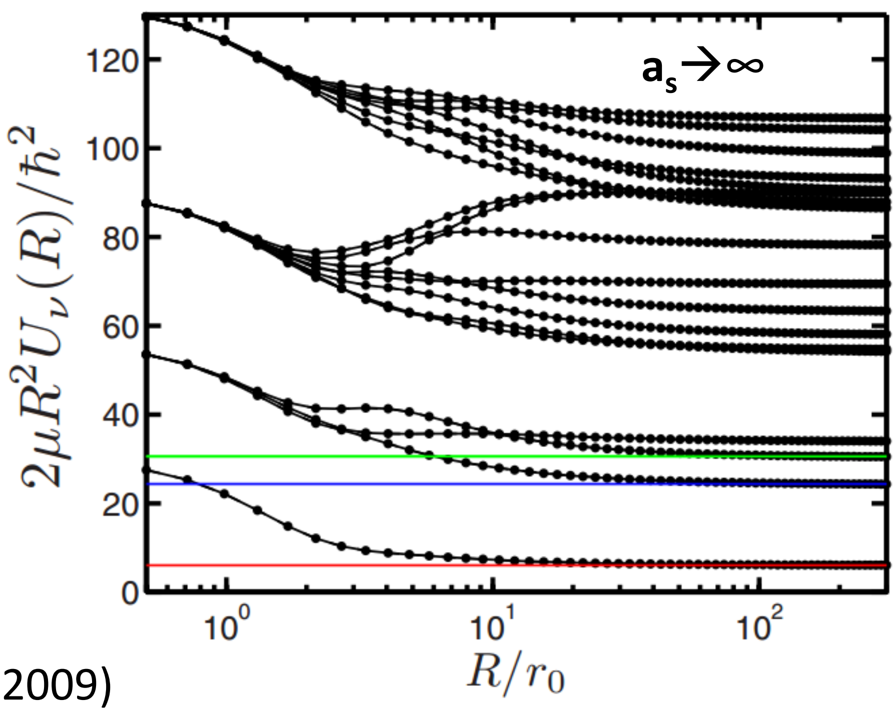
3. **Perform one more integration analytically.**
4. **Perform N-2 remaining numerical integrations.**

von Stecher and Greene, Phys. Rev. A **80**, 022504 (2009);
Rittenhouse *et. al.,* J. Phys. B: At. Mol. Opt. Phys. **44** 172001 (2011);
Rakshit and Blume, Phys. Rev. A **86**, 062513 (2012);

First use of HECG: Gaussian interactions



$$V_{\text{int}} = \sum_{i<j} V_0 \exp\left(-\frac{1}{2}\frac{|\boldsymbol{r}_i - \boldsymbol{r}_j|^2}{r_0^2}\right)$$



von Stecher and Greene, Phys. Rev. A **80**, 022504 (2009)

Matrix element strategy: new approach

(same example as last slide)

Daily and Greene PRA.89.012503.2014

$$\langle A|A'\rangle_{\boldsymbol{\Omega}} = \int \exp\left(-\tfrac{1}{2}R_0^2 f_A(\boldsymbol{\Omega})\right)\exp\left(-\tfrac{1}{2}R_0^2 f_{A'}(\boldsymbol{\Omega})\right) d\boldsymbol{\Omega}$$

$$= \int \exp\left(-\tfrac{1}{2}R_0^2\left[f_A(\boldsymbol{\Omega}) + f_{A'}(\boldsymbol{\Omega})\right]\right) d\boldsymbol{\Omega}$$

Trick #1

$$= \int \exp\left(-\tfrac{1}{2}R^2\left[f_A(\boldsymbol{\Omega}) + f_{A'}(\boldsymbol{\Omega})\right]\right) \underline{\delta(R_0^2 - R^2)} d\boldsymbol{\Omega} dR^2$$

$$= \frac{2}{R_0^{Nd-2}} \int \exp\left(-\tfrac{1}{2}R^2\left[f_A(\boldsymbol{\Omega}) + f_{A'}(\boldsymbol{\Omega})\right]\right) \delta(R_0^2 - R^2) R^{Nd-1} dR d\boldsymbol{\Omega}$$

$$= \frac{2}{R_0^{Nd-2}} \int \exp\left(-\tfrac{1}{2}\boldsymbol{x}^T[\underline{A} + \underline{A}']\boldsymbol{x}\right) \delta(R_0^2 - \boldsymbol{x}^T\boldsymbol{x}) d^{Nd}\boldsymbol{x}$$

Trick #2

$$\frac{1}{2\pi}\int \exp\left(\imath\omega(R_0^2 - \boldsymbol{x}^T\boldsymbol{x})\right) d\omega$$

$$= \frac{1}{\pi R_0^{Nd-2}} \iint \exp\left(-\tfrac{1}{2}\boldsymbol{y}^T\left[\underline{D} + 2\imath\omega\underline{1}\right]\boldsymbol{y}\right) \exp\left(\imath\omega R_0^2\right) d^{Nd}\boldsymbol{y}\, d\omega$$

Switch to coordinates that diagonalize A+A'

$$= \frac{(2\pi)^{Nd/2}}{\pi R_0^{Nd-2}} \int \exp\left(\imath\omega R_0^2\right) \prod_{j=1}^{N} (\gamma_j + 2\imath\omega)^{-d/2} d\omega$$

Matrix element strategy: final tricks

$$\frac{(2\pi)^{(Nd+1)/2}}{\pi t^{Nd/2-1}} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(\imath\omega t) \prod_{j=1}^{N} (\gamma_j + 2\imath\omega)^{-d/2} d\omega$$

$t=R_0^2$

If d is even, then can use contour integration.

For any d, can use convolution theorem.

$$\frac{(2\pi)^{(Nd+1)/2}}{\pi t^{Nd/2-1}} \left[f_{\gamma_1}^{d/2} * f_{\gamma_2}^{d/2} * \cdots * f_{\gamma_N}^{d/2} \right](t)$$

$$\left[f_{\gamma_1}^{k_1} * f_{\gamma_2}^{k_2} \right](t) = \frac{1}{\sqrt{2\pi}} \int_0^t f_{\gamma_1}^{k_1}(s) f_{\gamma_2}^{k_2}(t-s) ds$$

Integration range restricted due to range of $t=R_0^2$

$$f_\gamma^k(t) = \sqrt{2\pi} \frac{t^{k-1}}{2^k \Gamma(k)} \exp\left(-\frac{1}{2}\gamma t\right)$$

Tricks vs technique

After all convolutions we have…

N>3 almost 1F1 function

$$\frac{2\pi^{(Nd)/2}}{\Gamma(Nd/2)} \exp\left(-\frac{1}{2}\gamma_N t\right) \sum_{s=0}^{\infty} \frac{([Nd-1]/2)_s}{(Nd/2)_s} \frac{[(\gamma_N - \gamma_{N-1})t/2]^s}{s!} C_s^{(3)}$$

Volume element of Nd-dimensional sphere

where the weight C_s is just a polynomial:

$$C_s^{(k)} = \sum_{r=0}^{s} \frac{([Nd-k+1]/2)_r}{([Nd-k+2]/2)_r} \left[\frac{\gamma_{N-k+2} - \gamma_{N-k+1}}{\gamma_{N-k+3} - \gamma_{N-k+2}}\right]^r \binom{s}{r} C_r^{(k+1)}$$

No t-dependence in the remaining polynomial and positive definite terms!

Table 7.1. Matrix elements, $\mathcal{M} = \langle g(\boldsymbol{s}'; A', \boldsymbol{x})|\mathcal{O}|g(\boldsymbol{s}; A, \boldsymbol{x})\rangle$, of operators $\mathcal{O}$ between generating functions g of Eq. (6.19). Here we take all vectors d-dimensional. $\tilde{w}\boldsymbol{x}$ is a short-hand notation for $\sum_{i=1}^{N} w_i \boldsymbol{x}_i$. A vector product $(\boldsymbol{a} \times \boldsymbol{b})$ and a tensor product $[\boldsymbol{a} \times \boldsymbol{b}]_{2\mu}$ are defined for three-dimensional vectors $\boldsymbol{a}$ and $\boldsymbol{b}$. $B = A + A'$, $\boldsymbol{v} = \boldsymbol{s} + \boldsymbol{s}'$ and $\boldsymbol{y} = A'B^{-1}\boldsymbol{s} - AB^{-1}\boldsymbol{s}'$. P is a permutation operator and the matrix T_P is defined by $P\boldsymbol{x} = T_P\boldsymbol{x}$.

$\mathcal{O}$	$\mathcal{M}$
1	$\mathcal{M}_0 \equiv \left(\frac{(2\pi)^N}{\det B}\right)^{\frac{d}{2}} \exp(\frac{1}{2}\tilde{\boldsymbol{v}}B^{-1}\boldsymbol{v})$
$\tilde{w}\boldsymbol{x}$	$\tilde{w}B^{-1}\boldsymbol{v}\mathcal{M}_0$
$\tilde{\boldsymbol{x}}Q\boldsymbol{x}$ (Q: a symmetric matrix)	$\left\{d\mathrm{Tr}(B^{-1}Q) + \tilde{\boldsymbol{v}}B^{-1}QB^{-1}\boldsymbol{v}\right\}\mathcal{M}_0$
$\left(\tilde{w}\boldsymbol{x} \times \tilde{\zeta}\boldsymbol{x}\right)$	$\left(\tilde{w}B^{-1}\boldsymbol{v} \times \tilde{\zeta}B^{-1}\boldsymbol{v}\right)\mathcal{M}_0$
$[\tilde{w}\boldsymbol{x} \times \tilde{\zeta}\boldsymbol{x}]_{2\mu}$	$[\tilde{w}B^{-1}\boldsymbol{v} \times \tilde{\zeta}B^{-1}\boldsymbol{v}]_{2\mu}\mathcal{M}_0$
$\tilde{\zeta}\boldsymbol{\pi}$ ($\boldsymbol{\pi}_j = -i\hbar\frac{\partial}{\partial \boldsymbol{x}_j}$)	$-i\hbar\tilde{\zeta}\boldsymbol{y}\mathcal{M}_0$
$\tilde{\boldsymbol{\pi}}\Lambda\boldsymbol{\pi}$ (Λ: a symmetric matrix)	$\hbar^2\left\{d\mathrm{Tr}(AB^{-1}A'\Lambda) - \tilde{\boldsymbol{y}}\Lambda\boldsymbol{y}\right\}\mathcal{M}_0$
L_z ($\hbar\boldsymbol{L} = \sum_i(\boldsymbol{x}_i \times \boldsymbol{\pi}_i)$)	$-i\sum_{ij}(B^{-1})_{ij}(\boldsymbol{s}'_i \times \boldsymbol{s}_j)_z\mathcal{M}_0$
$\boldsymbol{L}^2$	$\left\{(d-1)\tilde{\boldsymbol{s}}'B^{-1}\boldsymbol{s} - \left(\sum_{ij}(B^{-1})_{ij}\boldsymbol{s}'_i \times \boldsymbol{s}_j\right)^2\right\}\mathcal{M}_0$
$\left(\tilde{w}\boldsymbol{x} \times \tilde{\zeta}\boldsymbol{\pi}\right)$	$-i\hbar\left(\tilde{w}B^{-1}\boldsymbol{v} \times \tilde{\zeta}\boldsymbol{y}\right)\mathcal{M}_0$
$\delta(\tilde{w}\boldsymbol{x} - \boldsymbol{r})$	$\mathcal{M}_1 \equiv (2\pi\tilde{w}B^{-1}w)^{-\frac{d}{2}} \times \exp\left\{-\frac{1}{2\tilde{w}B^{-1}w}(\boldsymbol{r} - \tilde{w}B^{-1}\boldsymbol{v})^2\right\}\mathcal{M}_0$
$\delta(\tilde{w}\boldsymbol{x} - \boldsymbol{r})\left(\tilde{w}\boldsymbol{x} \times \tilde{\zeta}\boldsymbol{\pi}\right)$	$-i\hbar\left\{\left(\boldsymbol{r} \times \tilde{\zeta}\boldsymbol{y}\right) + \frac{\tilde{\zeta}AB^{-1}w}{\tilde{w}B^{-1}w}\left(\boldsymbol{r} \times \tilde{w}B^{-1}\boldsymbol{v}\right)\right\}\mathcal{M}_1$
P	$\langle g(\boldsymbol{s}'; A', \boldsymbol{x}) \vert g(\widetilde{T_P}\boldsymbol{s}; \widetilde{T_P}AT_P, \boldsymbol{x})\rangle$

Can "translate" matrix elements that have already been calculated using the traditional ECG method.

Puts HECG method on approximately equal footing with tradiational ECG.

Suzuki and Varga, *Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems*, 1998.

Mitroy *et al.*, Rev. Mod. Phys. **85**, 693 (2013)

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Evidence for the Formation of Positronium in Gases*

MARTIN DEUTSCH
Laboratory for Nuclear Science and Engineering, and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts

(Received March 13, 1951)

VOLUME 46, NUMBER 11 PHYSICAL REVIEW LETTERS 16 MARCH 1981

Observation of the Positronium Negative Ion

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Bell Laboratories, Murray Hill, New Jersey 07974

(Received 24 December 1980)

Vol 449 | 13 September 2007 | doi:10.1038/nature06094 nature

LETTERS

The production of molecular positronium

D. B. Cassidy[1] & A. P. Mills Jr[1]

- o-Ps (S=1): 142ns → 3 gamma rays (C=-1)
- p-Ps (S=0): 125ps → 2 gamma rays (C=+1)

$$\text{o-Ps} + \text{o-Ps} \leftrightarrow \text{p-Ps} + \text{p-Ps} + 2E_\text{h}$$

$$X + \text{o-Ps} + \text{o-Ps} \leftrightarrow X + \text{Ps}_2 + E_\text{b}$$

Cassidy and Mills, Nat. Lett. **449**, 060904 (2009)

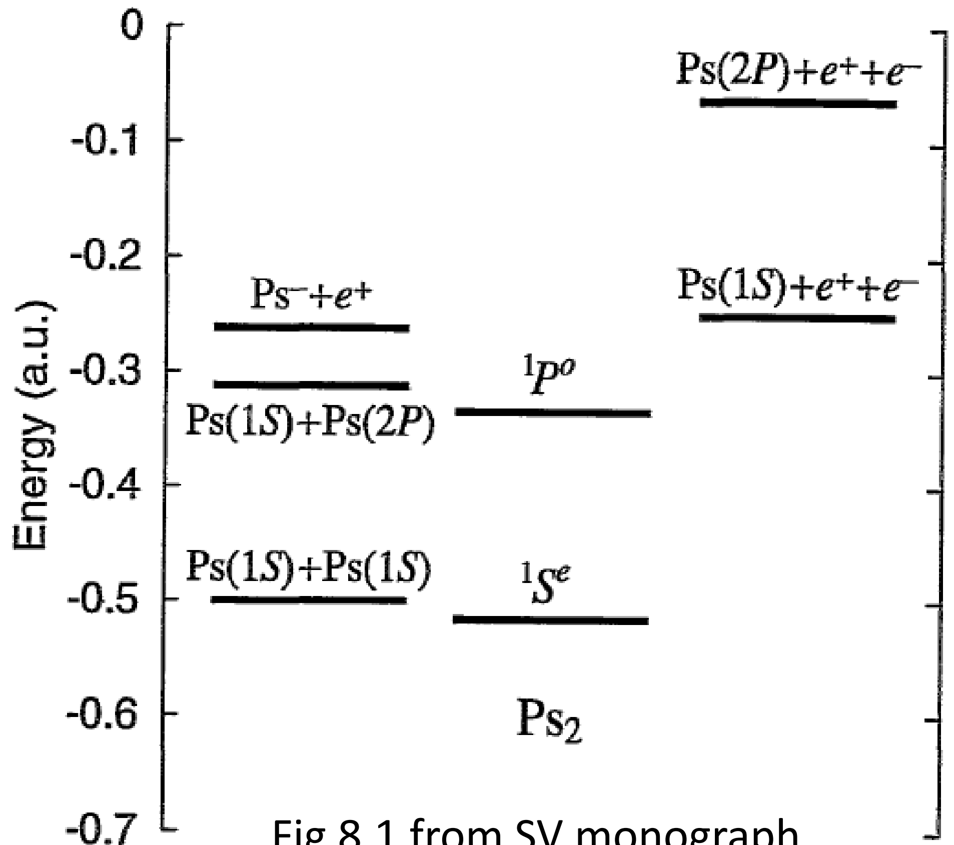

Fig 8.1 from SV monograph

Examples of polyelectronic complexes

TABLE XVIII. SVM energies of 2D and 3D excitonic complexes in hartree (Usukura, Suzuki, and Varga, 1999).

	2D		3D	
System	$E(\sigma = 0)$	$E(\sigma = 1)$	$E(\sigma = 0)$	$E(\sigma = 1)$
eh	−2.000	−1.000	−0.500	−0.250
eeh	−2.240	−1.121	−0.527	−0.262
ehh	−2.818	−1.121	−0.602	−0.262
eehh	−5.33	−4.385	−1.174	−0.516
eeehh	Unbound	Unbound	Unbound	Unbound
eehhh	−6.82	Unbound	−1.343	Unbound

σ=1: equal mass

σ=0: m_h >> m_e

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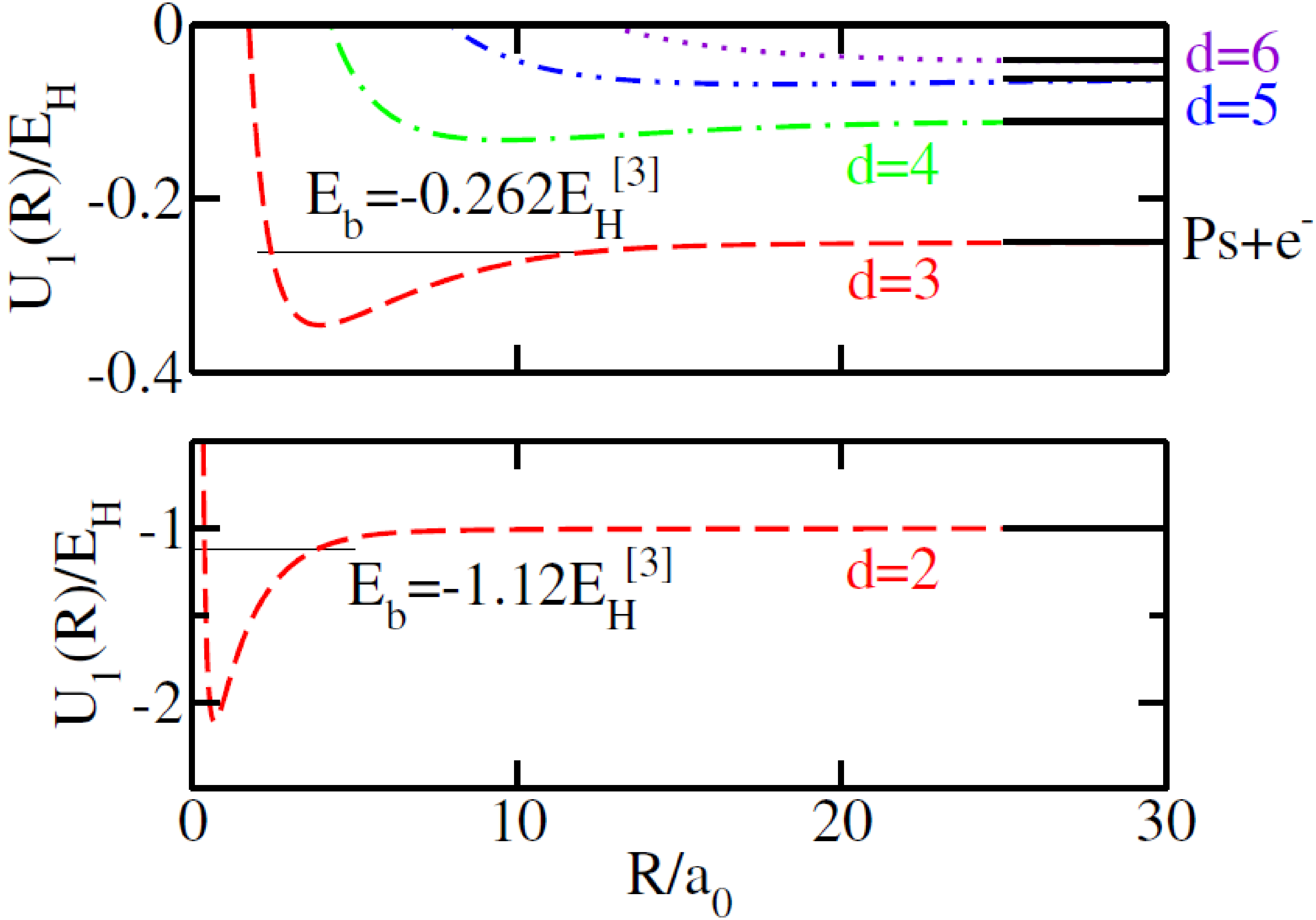
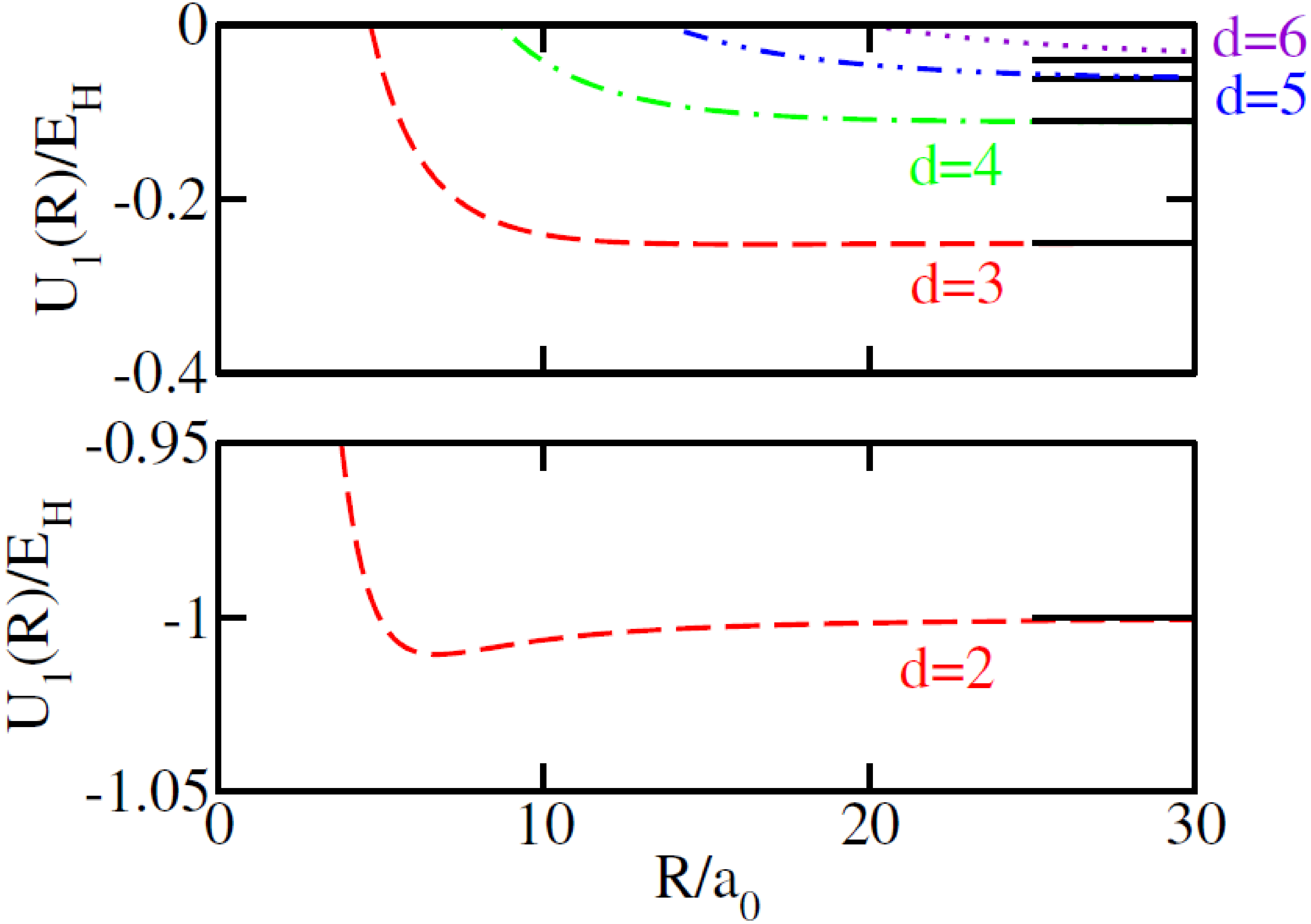
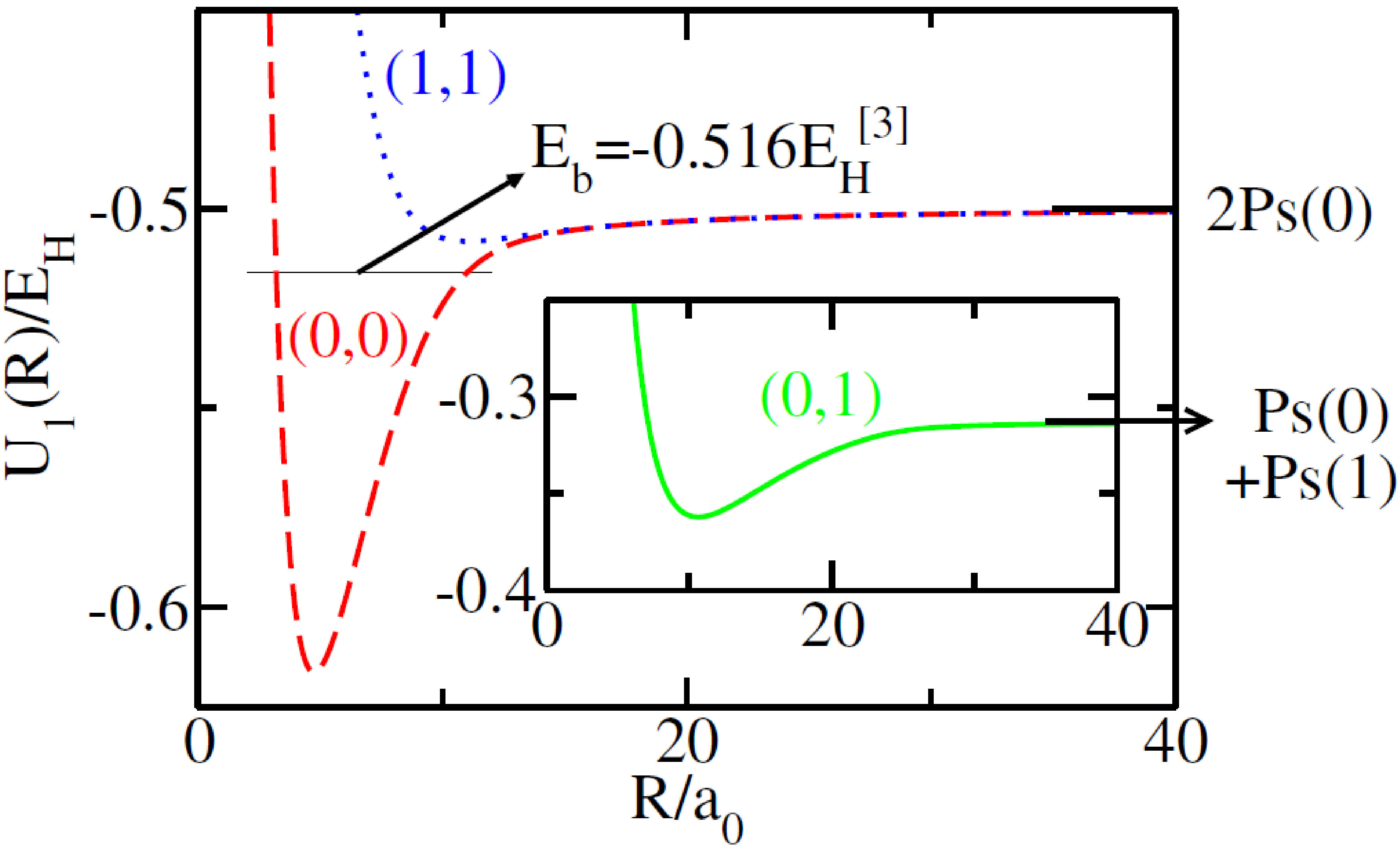
$(+)_1(-)_2$: $(S_+,S_-)=(1/2,0)$


0
-0.2
-0.4
$U_1(R)/E_H$
E_b=-0.262E_H[3]
d=6
d=5
d=4
Ps+e$^-$
d=3
-1
-2
E_b=-1.12E_H[3]
d=2
0
10
20
30
R/a_0

$(+)_1(-)_2$: $(S_+,S_-)=(1/2,1)$

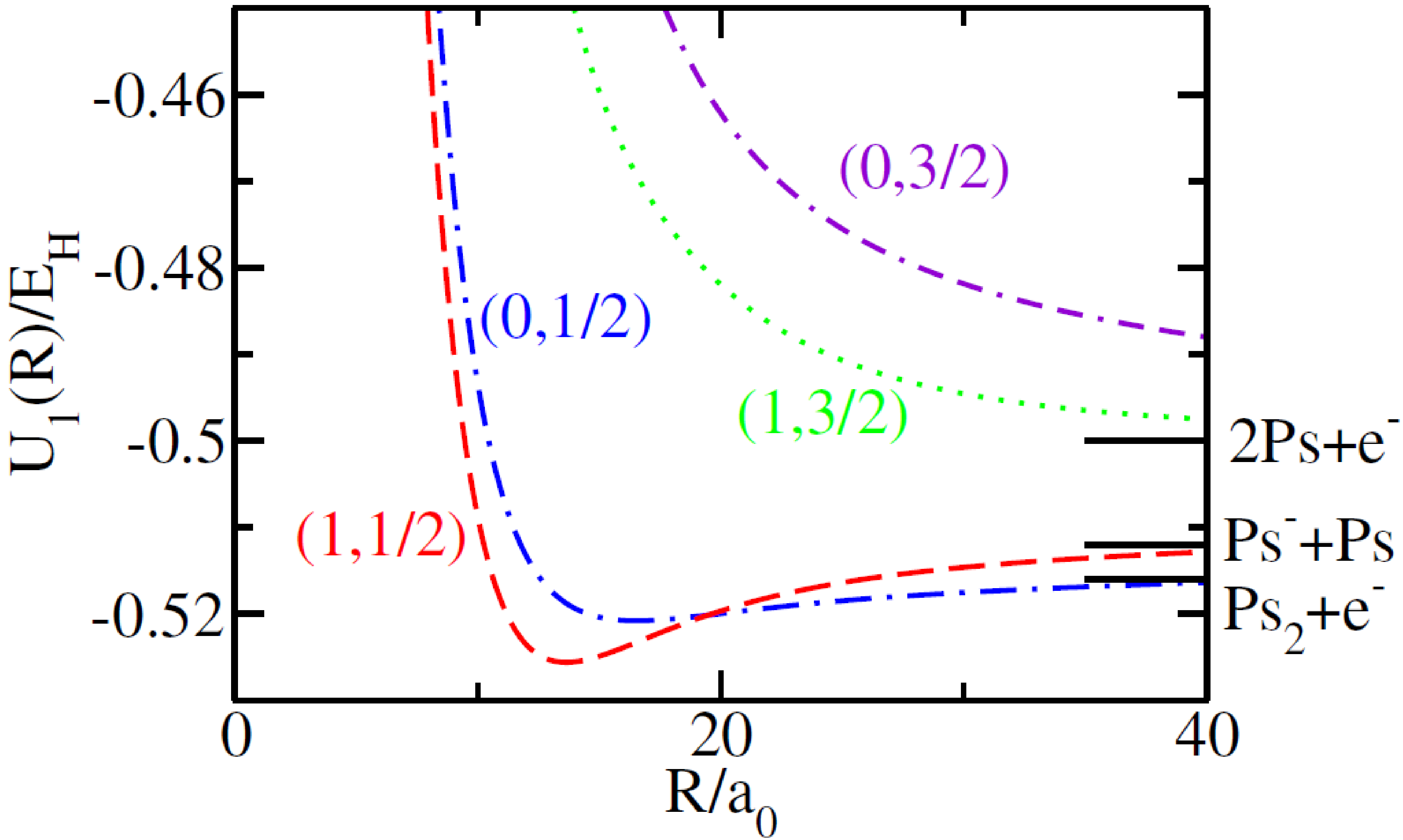


4-body: $(+)_2(-)_2$

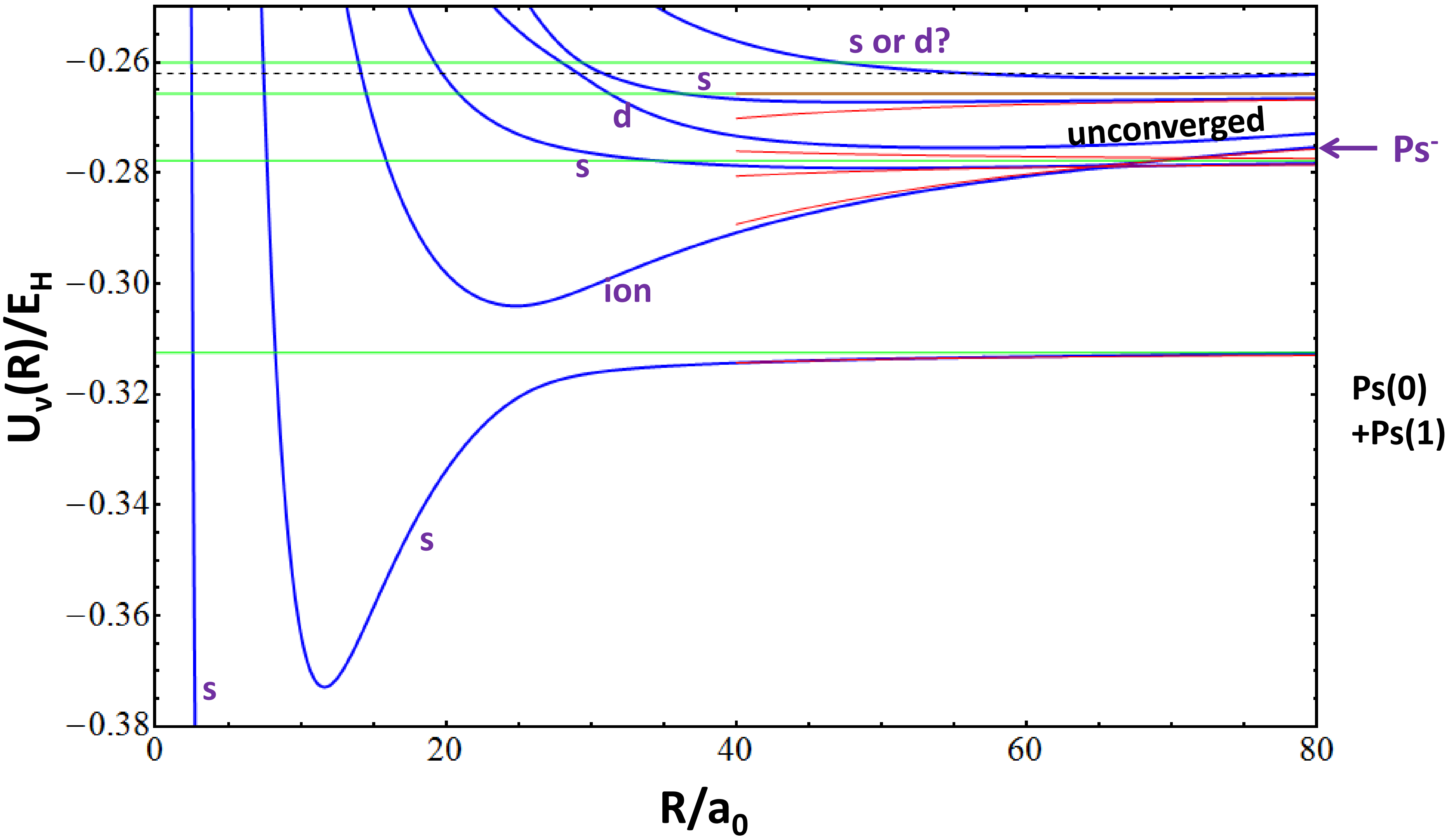


(1,1)
E_b=-0.516E_H^[3]
2Ps(0)
-0.5
-0.6
U_1(R)/E_H
(0,0)
(0,1)
-0.3
-0.4
0
20
40
Ps(0)
+Ps(1)
0
20
40
R/a_0

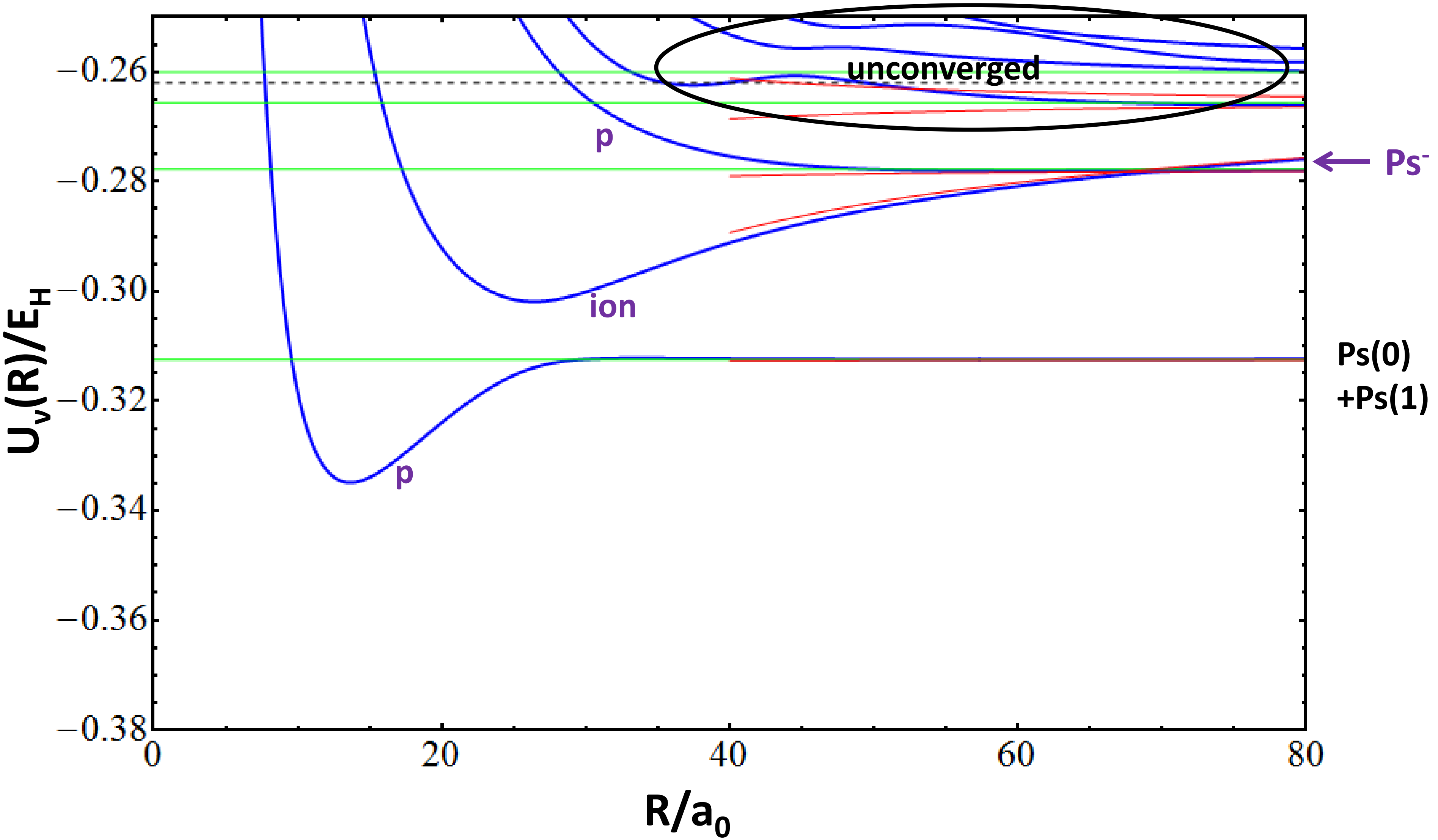
5-body: $(+)_2(-)_3$



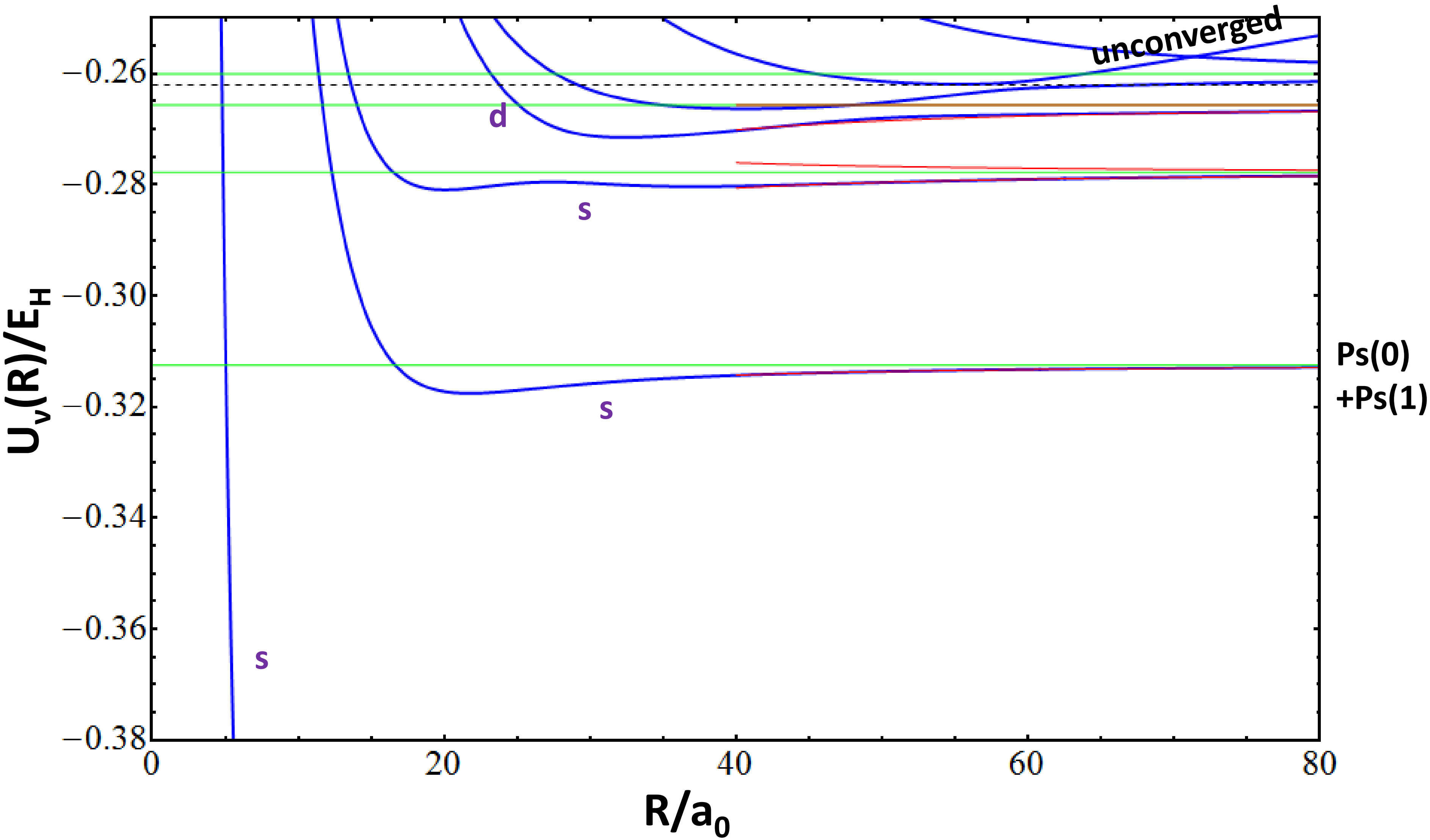
$(+)_2(-)_2$: $(S_+,S_-)=(0,0)$ and C=+1



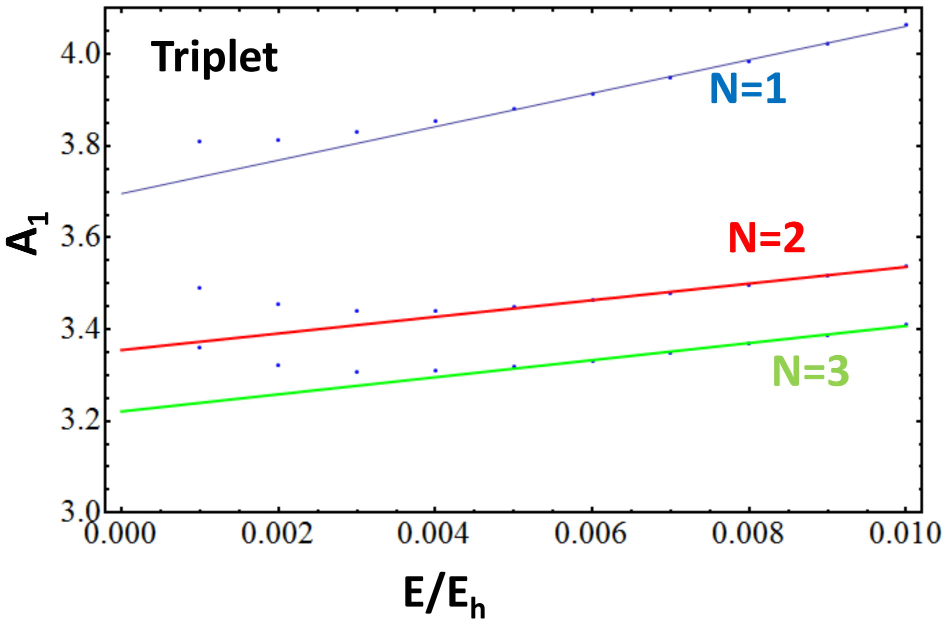
$(+)_2(-)_2$: $(S_+,S_-)=(0,0)$ and C=-1

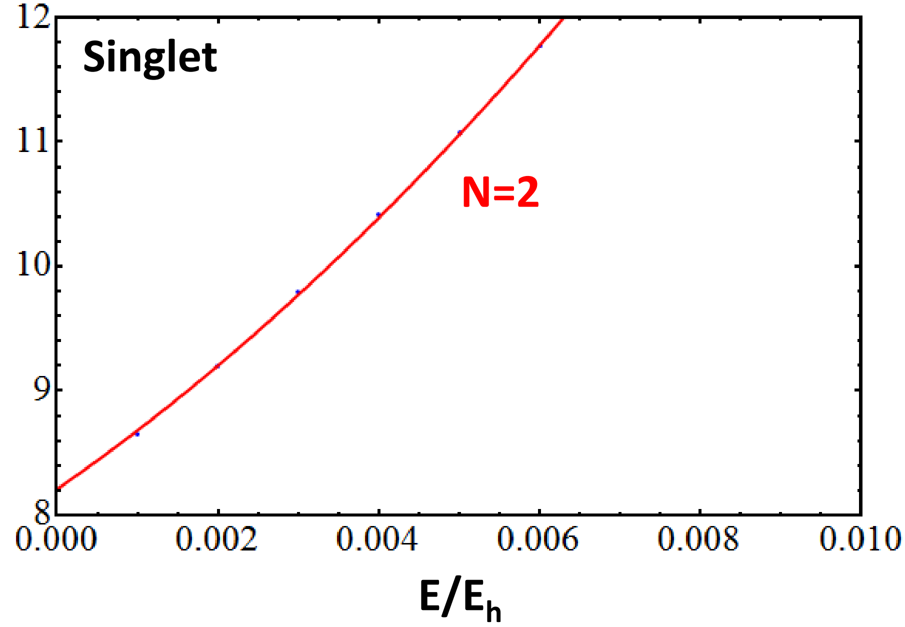


$(+)_2(-)_2$: $(S_+,S_-)=(1,1)$ and C=+1



Preliminary scattering data





We understand our deviations at small scattering energies and can correct them.

TABLE I. The scattering length and effective range (in a_0) for some calculations of Ps-Ps scattering. The present results are given to three significant figures after the decimal point purely for plotting purposes.

Method	Singlet		Triplet	
	A_0	r_0	A_1	r_1
Estimate from Ps_2 energy	5.59			
[a]Platzmann and Mills [12]	≈ 5.7		≈ 1.9	
[a]Oda *et al.* [9]	8.26	3.84	3.02	
Superseded SVM [20]	8.4		2.95	
Present SVM	8.443	4.761	2.998	2.247
QMC [25]	9.148 ± 0.042	-6.632	3.024 ± 0.058	1.729

[a]The triplet values are not the result of any calculation, but rather estimates based on physical insight about the nature of the collision.

Ivanov, Mitroy, Varga, Phys. Rev. A **65**, 022704 (2002).

Outlook

- **More thorough study of elastic and inelastic scattering.**
- **We can treat ion dissociation on equal footing to other processes.**
- **Ion pair formation rates.**
- **What can we learn about H_2 this way?**
- **2-D studies, e.g. Hall physics, “dropletons”, etc.**