Hyperspherical calculations for Coulomb three-body systems

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The hyperspherical (HS) approach has been applied to solve bound states and scattering problems in many different fields of physics and chemistry

My talk is on the HS calculations in atomic physics, particularly for three-body Coulomb systems.

The HS approach was applied to the study of doubly excited (resonance) states of helium and H^- in 1968. Then, for about two decades, HS approach had been used for conceptual and qualitative purposes.

Around 1990, computational techniques were developed to perform accurate calculations in HS coordinates. HS approach was extended to general three-body systems, and many studies have been made to obtain accurate quantitative results.

I will introduce the advantages of HS approach by explaining the theory and by showing numerical results.

Outlines

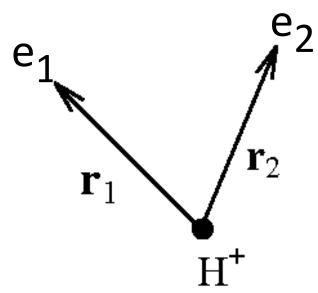
Theory

- Atomic orbital（AO) expansion for H^-
- Hyperspheical coupled-channel (HSCC) method for H^- , and for general three-body Coulomb systems

Application

H^-, $e^+ + He^+$, $He^{2+} + (p\,\mu)$, HD^+

Atomic-orbital (AO) expansion for H$^-$ system



$$\text{Hamiltonian } H = -\frac{1}{2}\nabla_1^2 - \frac{1}{r_1} - \frac{1}{2}\nabla_2^2 - \frac{1}{r_2} + \frac{1}{r_{12}}$$

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{n\ell m} \Big(F_{n\ell m}(\mathbf{r}_2)\ \varphi_{n\ell m}(\mathbf{r}_1) + (-1)^S F_{n\ell m}(\mathbf{r}_1)\ \varphi_{n\ell m}(\mathbf{r}_2) \Big)$$

$$\mathbf{L}^2 = (\mathbf{l}_1 + \mathbf{l}_2)^2, \quad \mathbf{S}^2 = (\mathbf{s}_1^2 + \mathbf{s}_2)^2, \ \ \Pi f(\mathbf{r}_1, \mathbf{r}_2) = f(-\mathbf{r}_1, -\mathbf{r}_2)$$

$$\text{Symmetry } \Gamma = \{L, S, \Pi\}$$

$$\textbf{AO expansion}, \ \ \Psi^\Gamma(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i=1}^{N} \left(\frac{f_i(r_2)}{r_2} \phi_i(\mathbf{r}_1, \hat{r}_2) + (-1)^S \frac{f_i(r_1)}{r_1} \phi_i(\mathbf{r}_2, \hat{r}_1) \right)$$

$$\textbf{Atomic-orbital basis}, \ \phi_i \equiv \phi_{n\ell l}(\mathbf{r}_1, \hat{r}_2) = R_{nl}(r_1)\ (Y_\ell(\mathbf{r}_1) \otimes Y_l(\mathbf{r}_2)_{LM_L}$$

$$\text{Inserting } (H - E)\Psi^\Gamma = 0,$$

$$\left(-\frac{1}{2} \left[\frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} \right] - \frac{k_i^2}{2} \right) f_i(r) + \sum_{j=1}^{N} \left(V_{ij}^D + (-1)^S V_{ij}^X \right) f_j(r) = 0$$

$$k_i^2/2 = E - \epsilon_i$$

$$\left(-\frac{1}{2}\left[\frac{d^2}{dr^2} - \frac{l_\mu(l_\mu+1)}{r^2}\right] - \frac{k_\mu^2}{2}\right) f_\mu(r) + \sum_{\nu=1}^{N} \left(V_{\mu\nu}^D + (-1)^S V_{\mu\nu}^X\right) f_\nu(r) = 0$$

$$\mathbf{F} = \begin{pmatrix} f_{11} & f_{12} & \dots & f_{1N} \\ f_{21} & f_{22} & \dots & f_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ f_{N1} & f_{N2} & \dots & f_{NN} \end{pmatrix} \quad f_{ij}, \quad i\text{-th channel}, \;\; j\text{-th solution}$$

$$\tilde{F} = \mathbf{FP}, \quad \mathbf{P}\text{: transformation matrix}$$

For scattering, $E > E_c$

open channel: $E - \epsilon_i = k_i^2/2 > 0$

$$f_{ij} \sim \frac{1}{\sqrt{k_i}} (\sin\theta_i \delta_{ij} + K_{ij}\cos\theta_i),$$

$$\theta_i = k_i r - l_i \pi/2$$

closed channel: $E - \epsilon_i < 0$

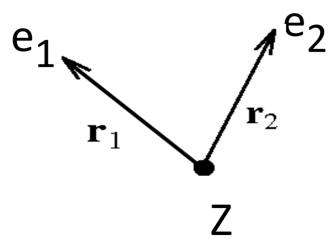
$$f_{ij} \sim e^{\kappa r}\delta_{ij} + K_{ij} e^{-\kappa r}$$

$$\mathbf{S} = (1 + i\mathbf{K})(1 - i\mathbf{K})^{-1}, \qquad \sum_i |S_{ij}|^2 = 1$$

In the single channel calculation, $K_{ii} = \tan\delta$, $S_{ii} = e^{2i\delta}$

For bound state, $E < E_c$ $\quad f_i \to 0 \quad (r \to \infty)$

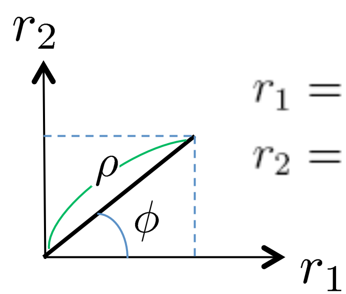
Hyperspheical coordinates for two-electro systems



$$\left(-\frac{1}{2}\nabla_1^2-\frac{1}{2}\nabla_2^2-\frac{Z}{r_1}-\frac{Z}{r_2}+\frac{1}{r_{12}}\right)\Psi(\mathbf{r}_1,\mathbf{r}_2)=E\Psi(\mathbf{r}_1,\mathbf{r}_2)$$

$$\rho=(r_1^2+r_2^2)^{1/2},\quad \phi=\tan^{-1}(r_2/r_1)$$

$$0\le\rho\le\infty,\quad 0\le\phi\le\pi/2$$



$$r_1=\rho\cos\phi,$$
$$r_2=\rho\sin\phi$$

$$\Psi=(\rho^{5/2}\sin\phi\cos\phi)^{-1}\overline{\Psi}$$

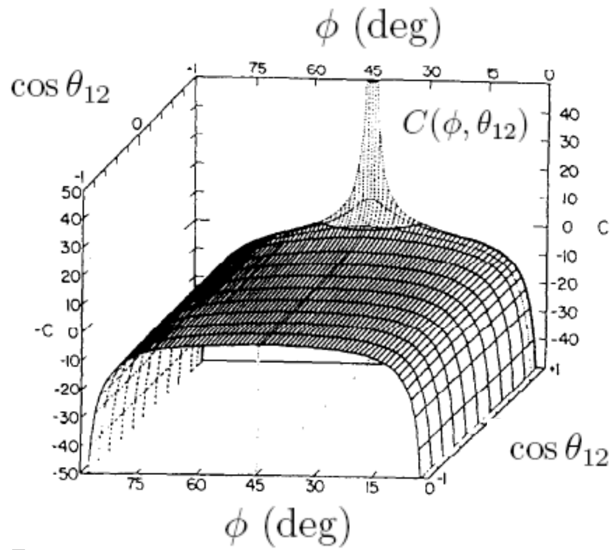
$$\left(-\frac{1}{2}\frac{\partial^2}{\partial\rho^2}+\underline{\frac{1}{2}\frac{\overline{\Lambda}^2(\Omega)}{\rho^2}+\frac{C(\phi,\theta_{12})}{\rho}}\right)\overline{\Psi}=E\overline{\Psi}$$

$$\overline{\Lambda}^2(\Omega)=-\frac{\partial^2}{\partial\phi^2}+\frac{\mathbf{l}_1^2}{\cos^2\phi}+\frac{\mathbf{l}_2^2}{\sin^2\phi}-\frac{1}{4}$$

$$C(\phi,\theta_{12})=-\frac{Z}{\cos\phi}-\frac{Z}{\sin\phi}+\frac{1}{\sqrt{1-\sin2\phi\cos\theta_{12}}}$$

$$\Omega=\{\phi,\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2\}$$

$$h_{ad}(\rho,\Omega)=\frac{1}{2}\frac{\overline{\Lambda}^2(\Omega)}{\rho^2}+\frac{C(\phi,\theta_{12})}{\rho}$$



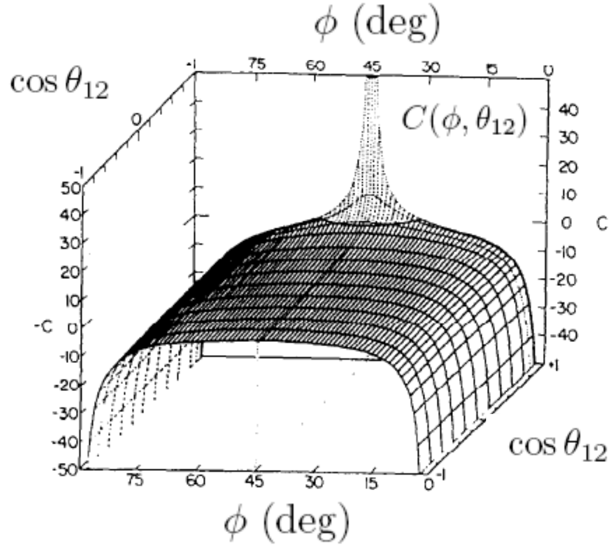
From
C.D. Lin, Phys. Rep. **257** pp1-83 (1995)

Adiabatic states

$$h_{ad}(\rho,\Omega) = \frac{1}{2}\frac{\overline{\Lambda}^2(\Omega)}{\rho^2} + \frac{C(\phi,\theta_{12})}{\rho}$$

$$h_{ad}(\rho,\Omega)\ \varphi_\mu(\rho,\Omega) = U_\mu(\rho)\ \varphi_\mu(\rho,\Omega),$$ $U_\mu(\rho)$: adiabatic potential

$\rho \to 0 \quad h_{ad}(\rho,\Omega) \sim \frac{1}{2}\frac{\overline{\Lambda}^2(\Omega)}{\rho^2}$



$\rho \to \infty,\ \phi \to 0\ , \quad r_2 \ll r_1 \simeq \rho$

$$h_{ad} \sim -\frac{1}{2}\left(\frac{\partial^2}{\partial r_2^2} - \frac{\mathbf{l}_2^2}{r_2^2}\right) - \frac{Z}{r_2} + O(1/\rho^2)$$

Variational bais for symmetry $\{L, M, S, \Pi\}$

$$(\cos\phi)^{l_1+1}(\sin\phi)^{l_2+1} f_{l_1 l_2 m}(\cos 2\phi)\mathcal{Y}^{LM}_{l_1 l_2}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2) + (-1)^S(1 \leftrightarrow 2),$$

$$(\cos\phi)^{l_1+1}(\sin\phi)^{l_2+1}\ r_2^n e^{-\alpha r_2}\mathcal{Y}^{LM}_{l_1 l_2}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2) + (-1)^S(1 \leftrightarrow 2)$$

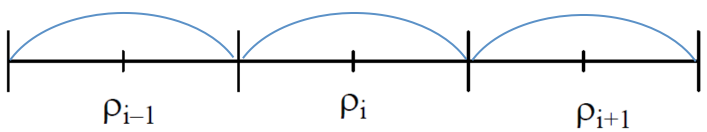
Hyperspherical coupled-channel equation

Adiabatic expansion: $$\overline{\Psi} = \sum_{\mu} F_\mu(\rho)\varphi_\mu(\Omega,\rho)$$

$$\left(\frac{d^2}{d\rho^2} + 2(E - U_\mu(\rho))\right) F_\mu(\rho) + \sum_\nu W_{\mu\nu}F_\nu(\rho) = 0,$$

$$W_{\mu\nu} = 2\left(\varphi_\mu \left| \frac{\partial}{\partial\rho} \varphi_\nu\right.\right) \frac{d}{d\rho} + \left(\varphi_\mu \left| \frac{\partial^2}{\partial\rho^2} \varphi_\nu\right.\right)$$

Piecewise diabatic expansion, diabatic-by-sector method.



$$\tilde{\Psi} = \sum_\mu F^i_\mu(\rho)\varphi^i_\mu(\Omega), \quad \varphi^i_\mu(\Omega) \equiv \varphi_\mu(\Omega,\rho_i).$$

$$\left(\frac{d^2}{d\rho^2} + 2E\right) F^i_\mu(\rho) - 2\sum_\nu \mathcal{V}_{\mu\nu}(\rho)F^i_\nu(\rho) = 0, \quad \mathcal{V}_{\mu\nu}(\rho) = \left(\varphi^i_\mu \left| h_{ad}(\rho,\Omega) \right| \varphi^i_\nu\right).$$

$$\begin{aligned} F^{i+1}_\mu(\rho_m) &= \sum_\nu \left(\varphi^{i+1}_\mu \left| \varphi^i_\nu\right.\right) F^i_\nu(\rho_m) \\ \frac{d}{d\rho}F^{i+1}_\mu(\rho_m) &= \sum_\nu \left(\varphi^{i+1}_\mu \left| \varphi^i_\nu\right.\right) \frac{d}{d\rho}F^i_\nu(\rho_m) \end{aligned} \quad (1)$$

Asymptotic solutions and matching at a large ρ

$$\Psi_j = (\rho^{5/2}\sin\phi\cos\phi)^{-1}\sum_\mu F_{\mu j}(\rho)\varphi_\mu$$

・・・ HS coordinates

$$= (\sqrt{2}r_>)^{-1}\sum_i \psi_i(\mathbf{r}_<, \hat{r}_>)\ [f_i(r_>)\delta_{ij} + g_i(r_>)K_{ij}]$$

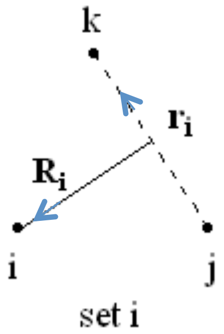
・・・ Independent coordinates $\mathbf{r}_1$, $\mathbf{r}_2$

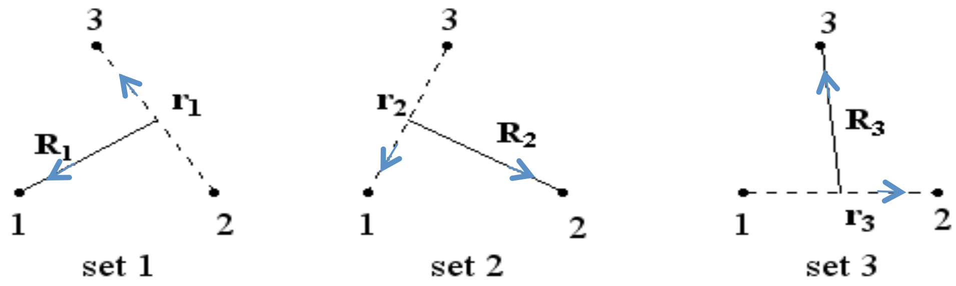
$$r_> = \max(r_1, r_2),\ \ r_< = \min(r_1, r_2)$$

$$r \to \infty \quad f_i(r) \sim \sin\theta_i/\sqrt{v_i}, \quad g_i(r) \sim \cos\theta_i/\sqrt{v_i}, \qquad \theta_i = k_i r - l_i\pi/2$$

ψ_i: atomic basis, K_{ij}: K-matrix

Hyperspherical coordinates for general three-body Coulomb systems





$$H = -\frac{1}{2M_i}\nabla^2_{R_i} - \frac{1}{2m_i}\nabla^2_{r_i} + \frac{z_1 z_3}{r_1} + \frac{z_3 z_1}{r_2} + \frac{z_1 z_2}{r_3}$$

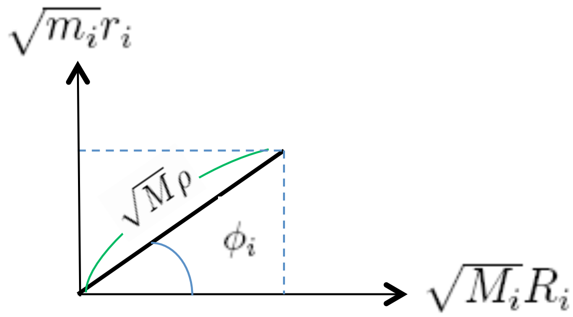
$$m_i = \frac{\mu_j \mu_k}{\mu_j + \mu_k}, \quad M_i = \frac{\mu_i(\mu_j + \mu_k)}{\mu_i + \mu_j + \mu_k}$$

$$M\rho^2 = M_i R_i^2 + m_i r_i^2$$

$$\phi_i = \tan^{-1}\frac{\sqrt{m_i} r_i}{\sqrt{M_i} R_i}$$

$$\Omega_i = \{\phi_i, \hat{\mathbf{r}}_i, \hat{\mathbf{R}}_i\}$$

$$\Omega_1 = \Omega_2 = \Omega_3 \equiv \Omega$$



$$\sqrt{M_i} R_i = \sqrt{M}\rho\cos\phi_i,$$
$$\sqrt{m_i} r_i = \sqrt{M}\rho\sin\phi_i.$$

$$H = -\frac{1}{2M}\left(\frac{d^2}{d\rho^2} + \frac{5}{\rho}\frac{d}{d\rho}\right) + h_{ad}(\rho,\Omega), \quad h_{ad} = \frac{1}{2M}\frac{\Lambda^2(\Omega)}{\rho^2} + V_C(\rho,\Omega)$$

$$\Lambda^2(\Omega_i) = -\frac{1}{\sin^2\phi_i\cos^2\phi_i}\left(\frac{d}{d\phi_i}\sin^2\phi_i\cos^2\phi_i\frac{d}{d\phi_i}\right) + \frac{\mathbf{l}_{R_i}^2}{\cos^2\phi_i} + \frac{\mathbf{l}_{r_i}^2}{\sin^2\phi_i},$$

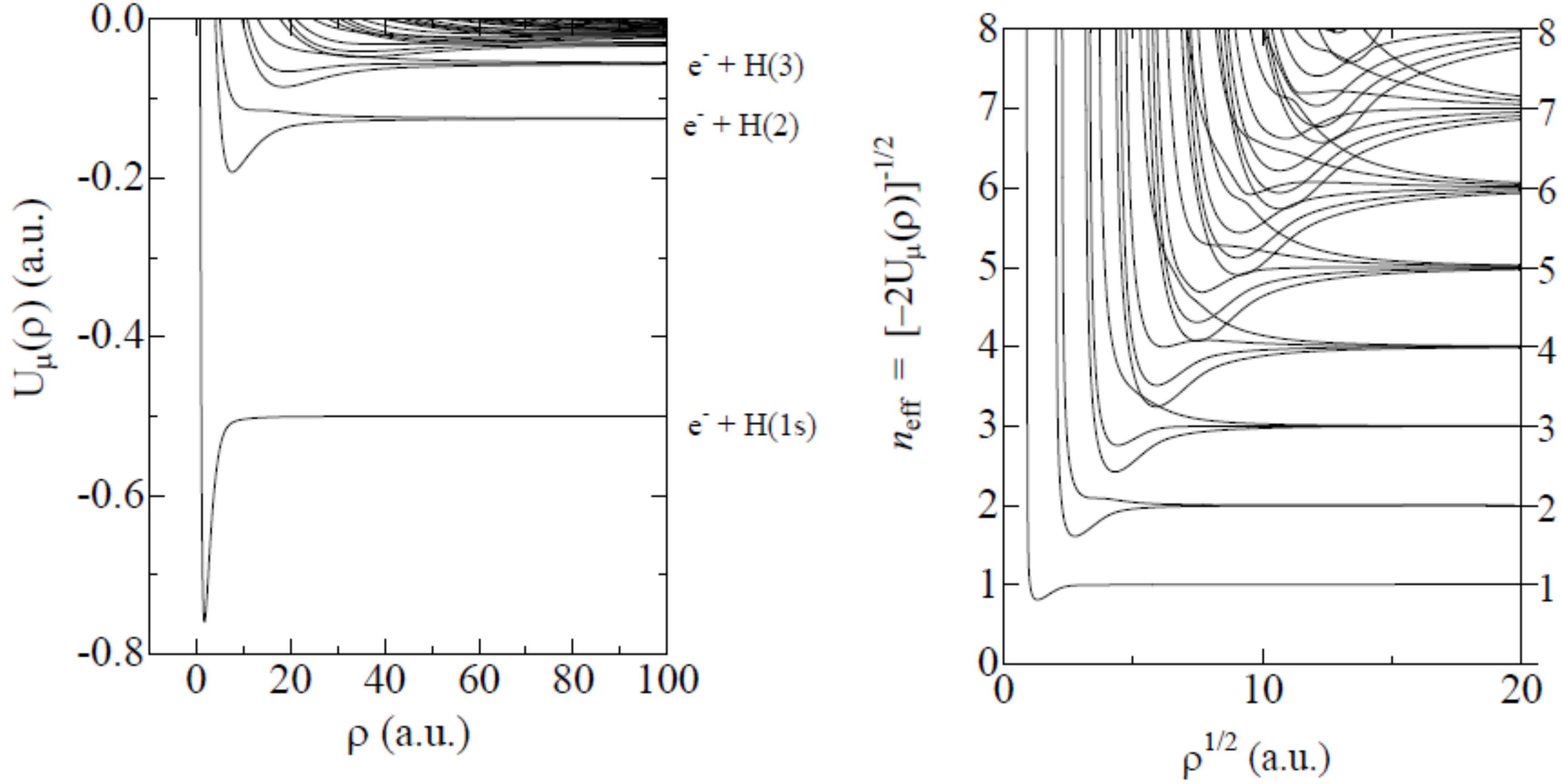
$$\Lambda^2(\Omega_1) = \Lambda^2(\Omega_2) = \Lambda^2(\Omega_3) \equiv \Lambda^2(\Omega)$$

$$h_{ad}(\Omega,\rho)\ \varphi_\mu(\Omega,\rho) = U_\mu(\rho)\ \varphi_\mu(\Omega,\rho)$$

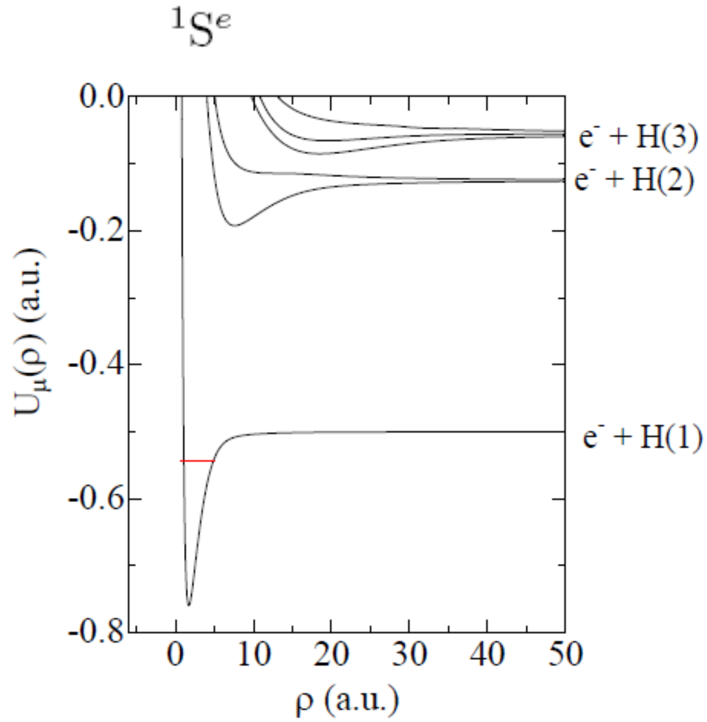
variational basis $\quad (\sin\phi_i)^\ell(\cos\phi_i)^l\ r_i^n e^{-\alpha r_i}\mathcal{Y}_{\ell l}^{LM}(\hat{\mathbf{r}}_i,\hat{\mathbf{R}}_i)$

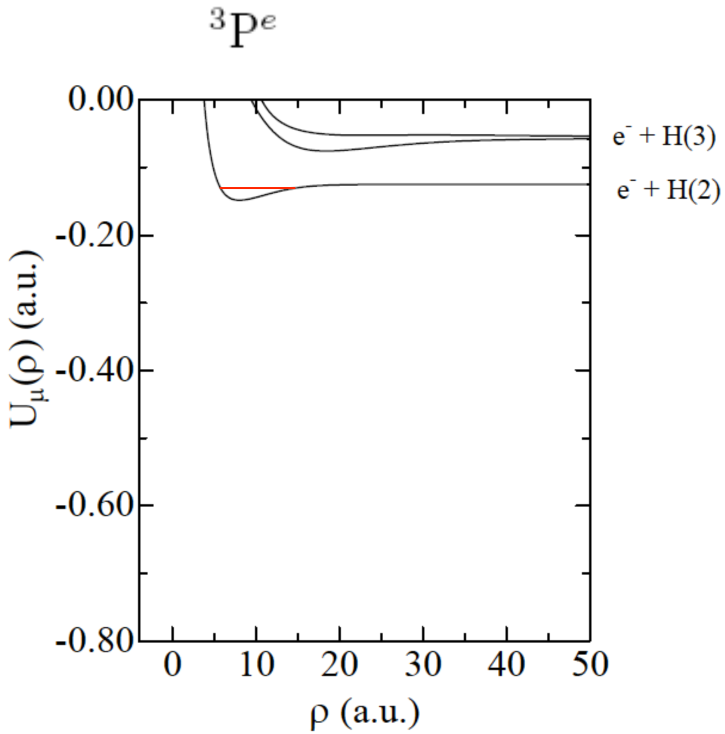
$$\Psi = \sum_\mu F_\mu(\rho)\varphi_\mu(\Omega,\rho)$$

Adiabatic potential curves for $^1S^e$ symmetry of H^-



Bound state calculation for H^-





The ground state energy
exact $-0.527\,75$

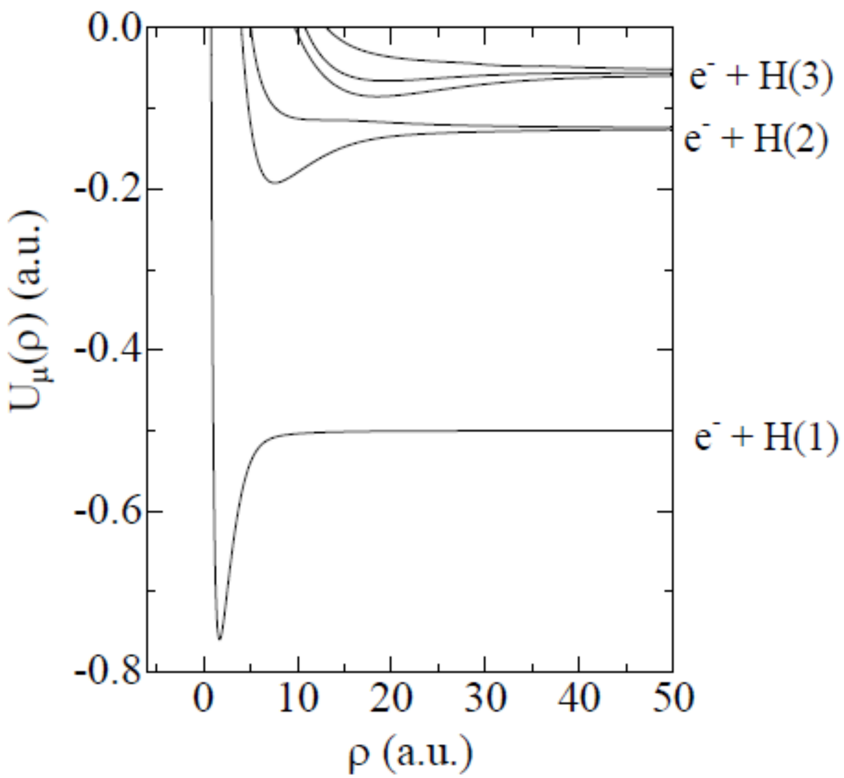
	HS	AO
$n = 1$	$-0.525\,91$	$-0.513\,31$
$n \leq 2$	$-0.527\,58$	$-0.522\,16$
$n \leq 3$	$-0.527\,60$	$-0.522\,92$

exact $-0.125\,35$

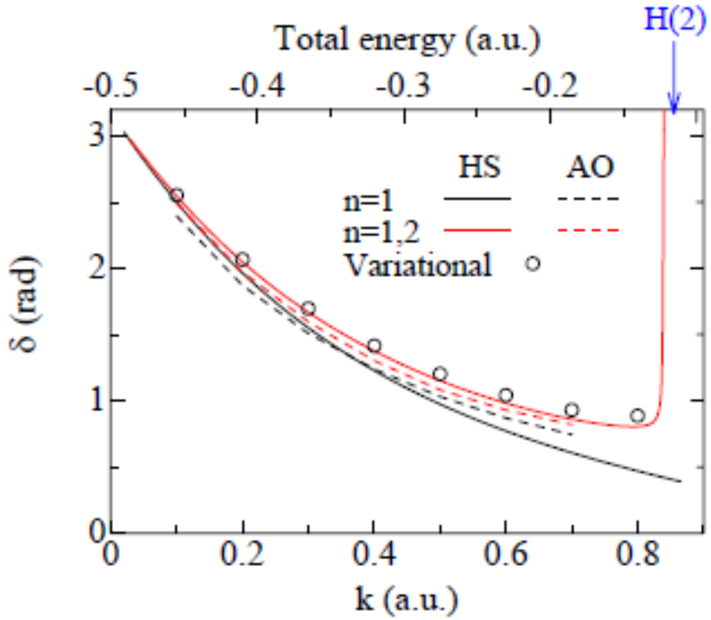
	HS	AO
$n \leq 2$	$-0.125\,10$	—
$n \leq 3$	$-0.125\,34$	$-0.125\,26$

$^1S^e$ phaseshift in $e^- + H(1s)$ scattering

Potential curves for
$^1S^e$ symmetry of H^-



$$E = k^2/2 - 0.5$$

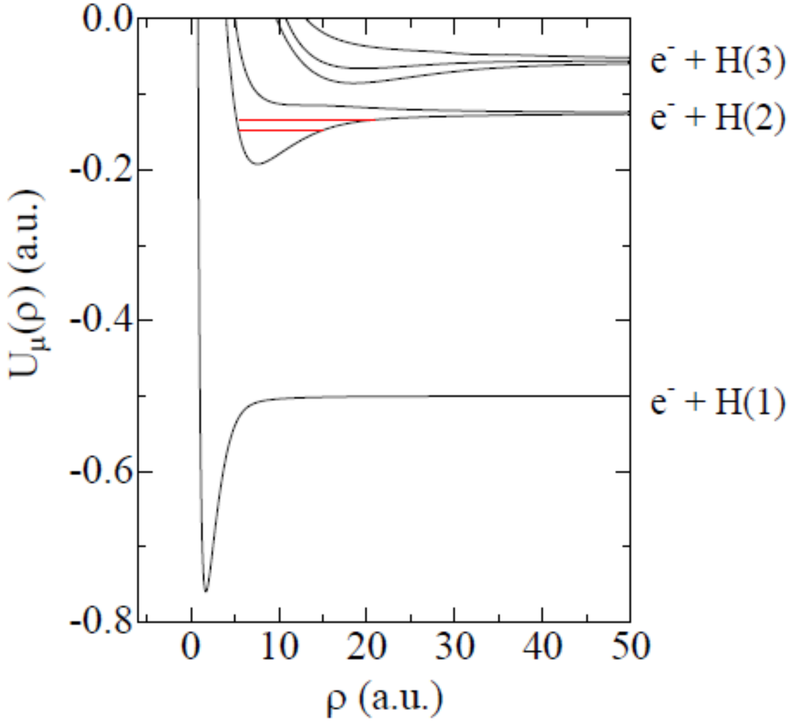


Resonance calculation

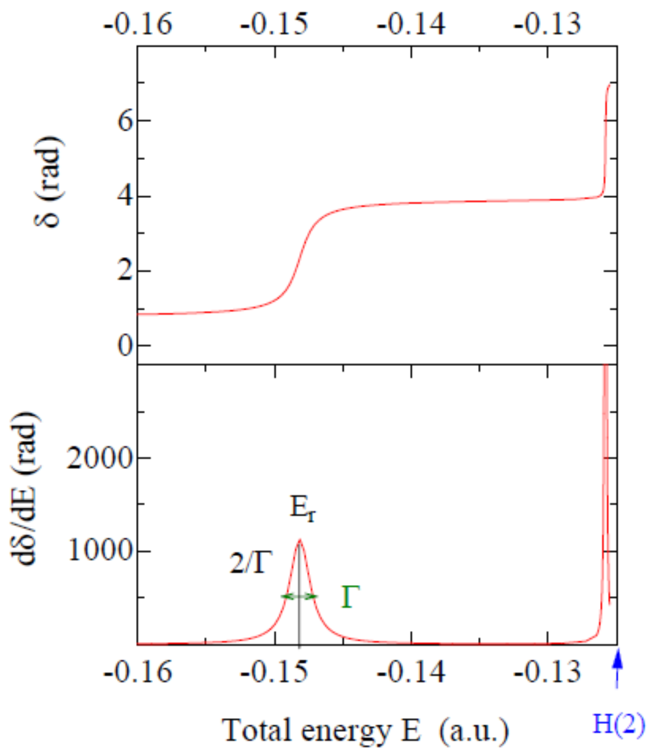
Breit-Wigner formula

$$\delta(E) = \tan^{-1}\frac{\Gamma/2}{E_r - E} + \delta_{bg}(E), \qquad \frac{d\delta(E)}{dE} = \frac{\Gamma/2}{(E-E_r)^2 + (\Gamma/2)^2} + \frac{d\delta_{bg}(E)}{dE}$$

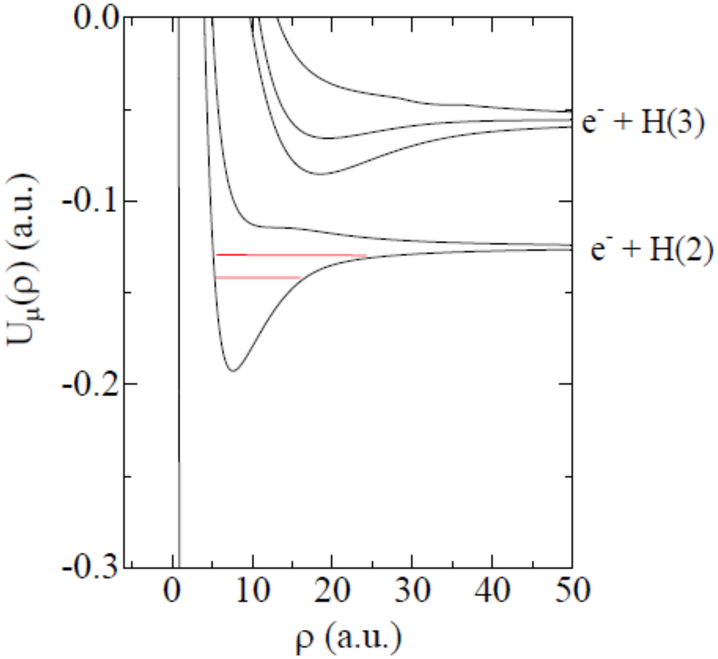
Potential curves for $^1S^e$ symmetry of H^-



$^1S^e$ phaseshift of $e^- + H(1s)$ scattering



Potential curves for $^1\mathrm{S}^e$ symmetry of H^-



Energy (E_r) and width (Γ) for the $^1\mathrm{S}^e$ resonances of H^- below the $\mathrm{H}(n=2)$ threshold

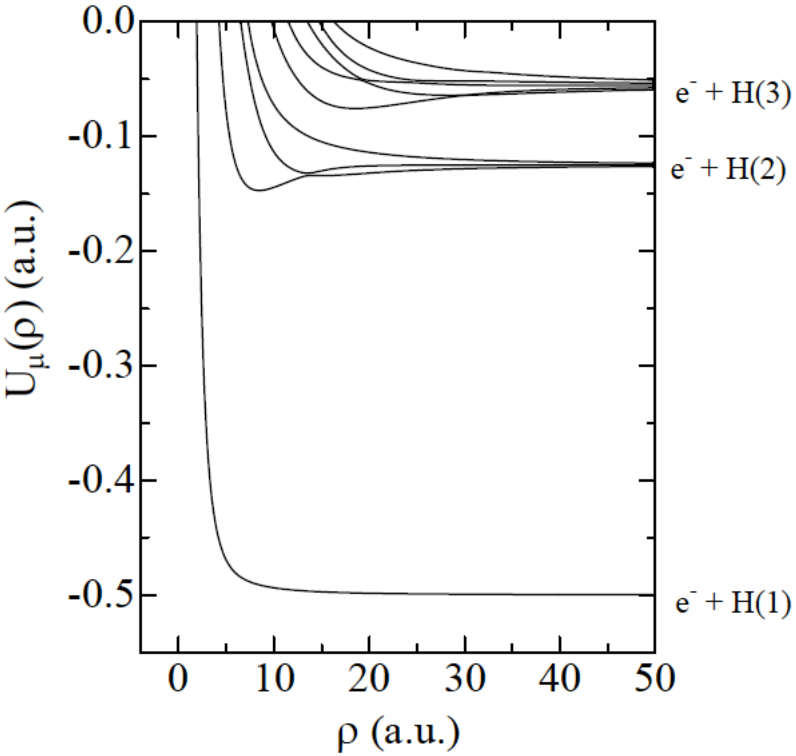
$^1\mathrm{S}^e(1)$

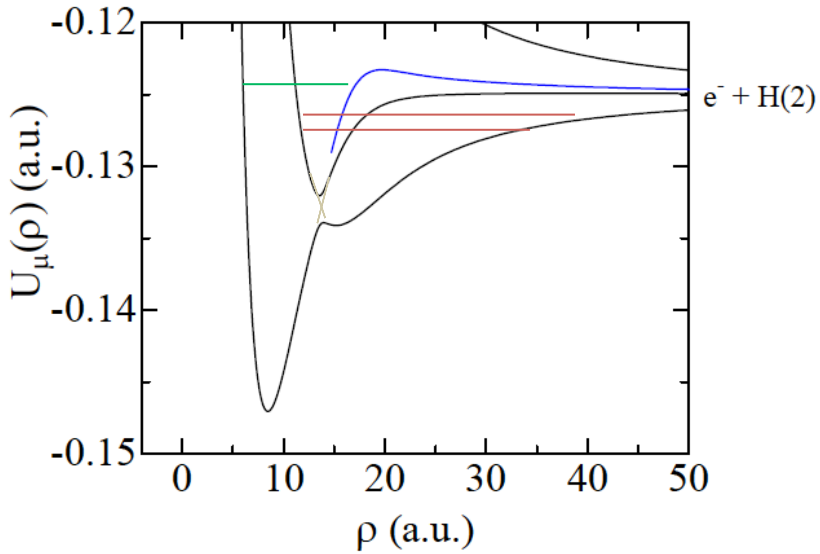
channels	(E_r , Γ)
1 channel	(−0.148 77, ———)
$n \le 2$	(−0.148 18, 1.8×10^{-3})
$n \le 3$	−0.148 76, 1.7×10^{-3})
Exp.	(−0.148 78, 1.7×10^{-3})

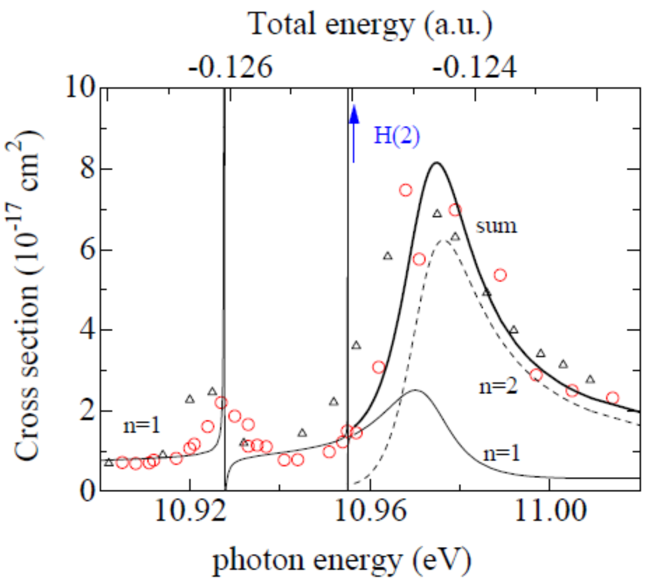
$^1\mathrm{S}^e(2)$

channels	(E_r , Γ)
1 channel	(−0.125 82, ———)
$n \le 2$	(−0.125 83, 7.2×10^{-5})
$n \le 3$	(−0.126 00, 8.6×10^{-5})

Potential curves for
$^1P^o$ symmetry of H^-





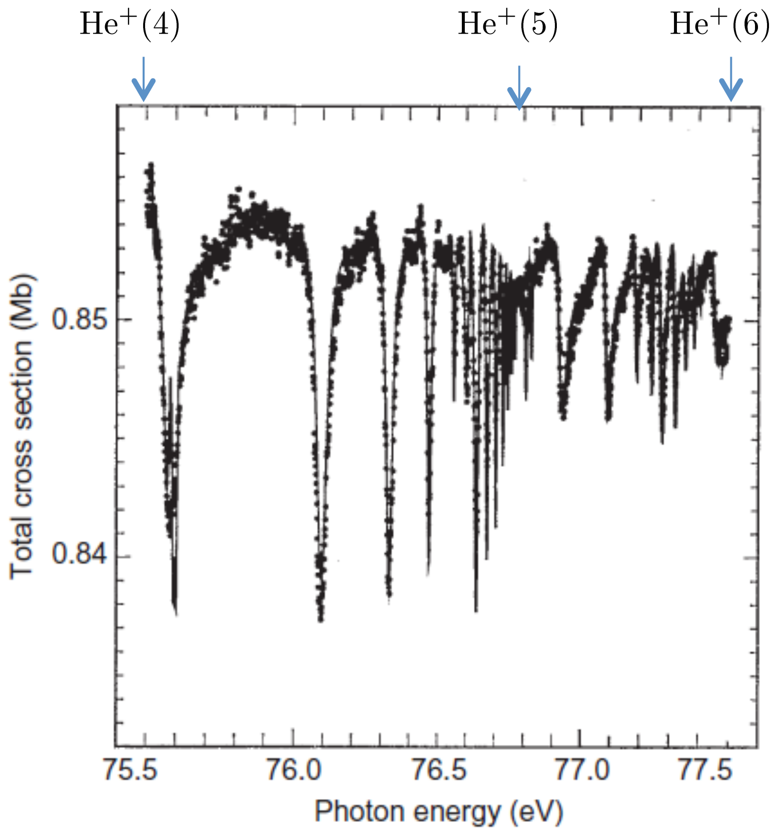


Photodetachment cross sections
of H^- near the $n = 2$ threshold

$$\hbar\omega + \mathrm{H}^-(1^1\mathrm{S}^e) \rightarrow e^- + \mathrm{H}(n)$$

Photoionization spectrum of $He(1^1S)$
for $He^+(n=4)$ and $He^+(n=6)$ thresholds.

$$\hbar\omega + \mathrm{He} \rightarrow e^- + \mathrm{He}^+$$



J.-Z. Tang and I. Shimamura,
Phys. Rev. A 50 (1994) 1321.

convoluted with an experimental energy resolution of 6 meV

Good points

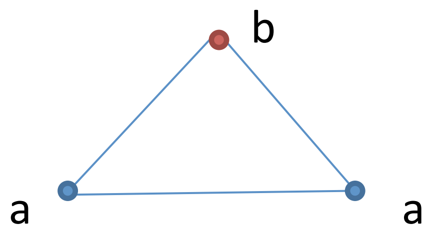
- Correlation among particles is considered in the adiabatic basis
- Potential curves give visual information on resonances
- Non-local potentials do not appear in the coupled radial equation.
- Convergence with respect to basis size is faster for a system where correlation among particles is strong
  => HS approach is strong for resonance calculations

Circumvented weak points

- Sharp change of non-adiabatic couplings near avoided crossing point
  => diabatic-by-sector method
- Adiabatic basis are not most suitable representation at large ρ
  => matching to atomic basis representation

HS treatment works irrespectively of mass combination

Systems including
two identical particles



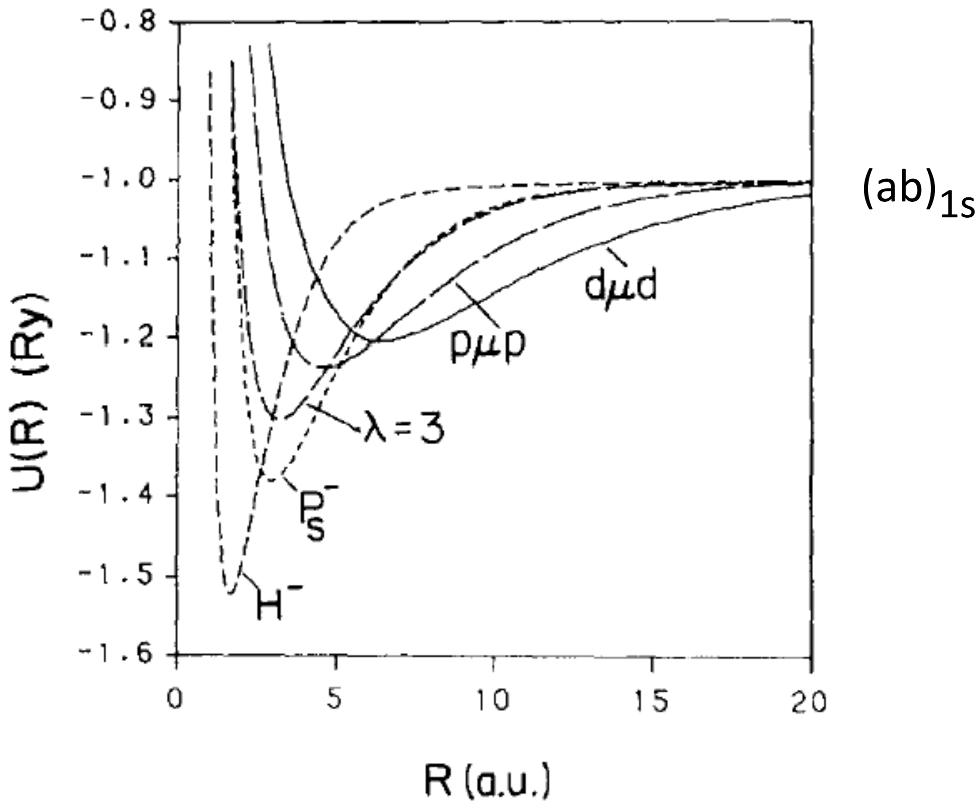
Mass ratio
$\lambda = m_a / m_b$

H^- ⟷ H_2^+

small — large

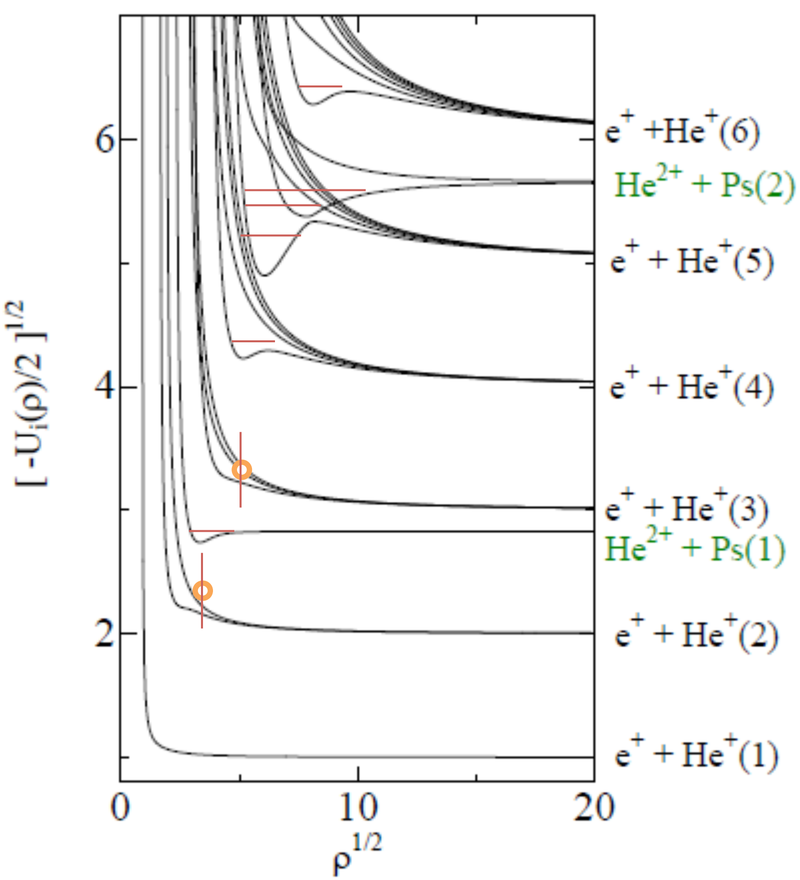
(1 bound state) — (18 bound states)

S-wave adiabatic potential curves of gerade symmetry for aba Coulomb three-body systems.



Z. Chen and C.D. Lin, Phys. Rev. A42, 18 (1990).

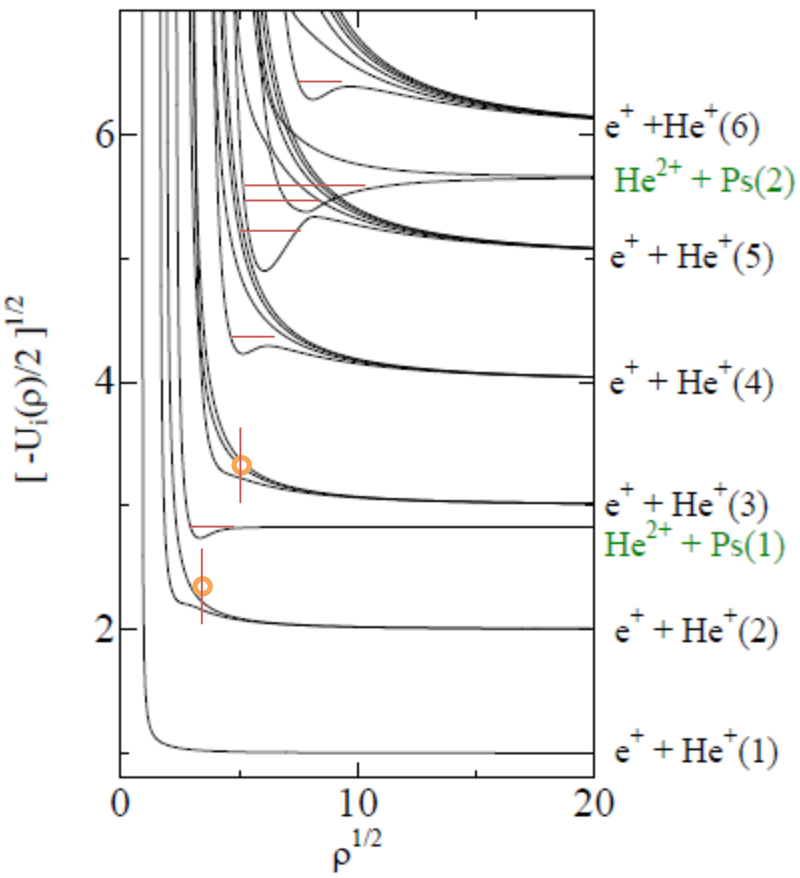
S-wave adiabatic potential curves of e^+He^+ system



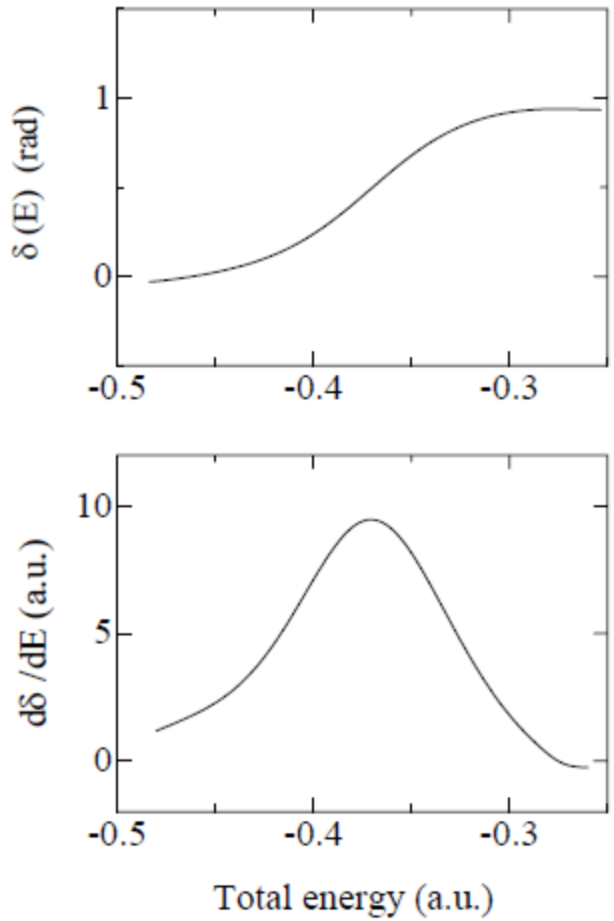
S-wave potential resoances in e^+He^+ system

level	HSSC	CRM
$He^+(7)$		
	$(-0.04755, 8.9[-4])$	
$He^+(6)$		
$Ps(2)$		
	$(-0.06431, 4.1[-4])$	$(-0.06433, 3.9[-4])$
	$(-0.06742, 7.3[-4])$	$(-0.06743, 7.9[-4])$
	$(-0.07539, 5.3[-4])$	$(-0.07540, 5.4[-4])$
	$(-0.1039, 5.0[-3])$	
$He^+(4)$		
	$(-0.188, 4.5[-2])$	$(-0.1856, 3.9[-2])$
$He^+(3)$		
$Ps(1)$		
	$(-0.25001, 7.[-6])$	
	$(-0.371, 1.4[-1])$	$(-0.3705, 1.3[-1])$
$He^+(2)$		

S-wave adiabatic potential curves of e^+He^+ system

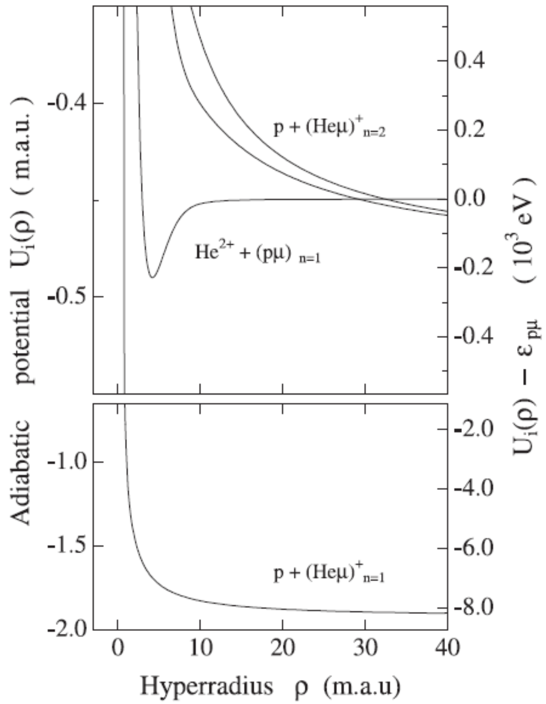


$\delta(E)$ and $\dfrac{d\delta(E)}{dE}$ for S-wave $e^+ + He^+$ scattering

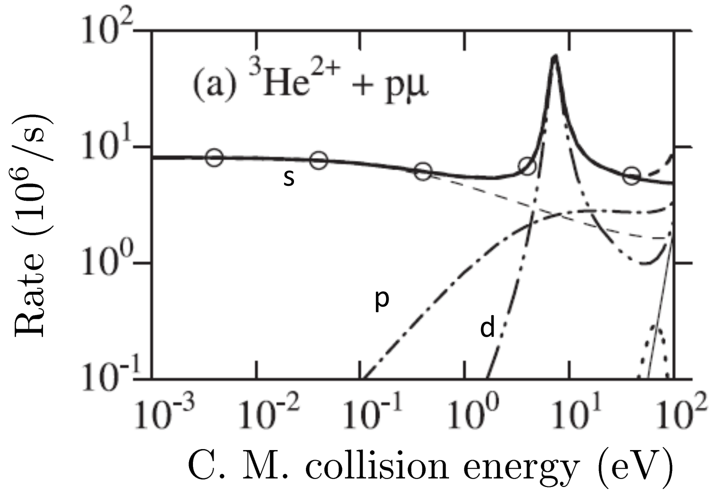


$$(x\mu)_{1s} + \mathrm{He} \to (x\mathrm{He}\mu) \to (\mathrm{He}\mu)_{1s} + x$$

S-wave adiabatic potential curves of $^3\mathrm{He}^{2+} + p\mu$ system



The muon transfer rates $(N_0 v\sigma)$ in $^3\mathrm{He}^{2+} + (p\mu)_{1s} \to (^3\mathrm{He}\mu)^+(n=1) + p$

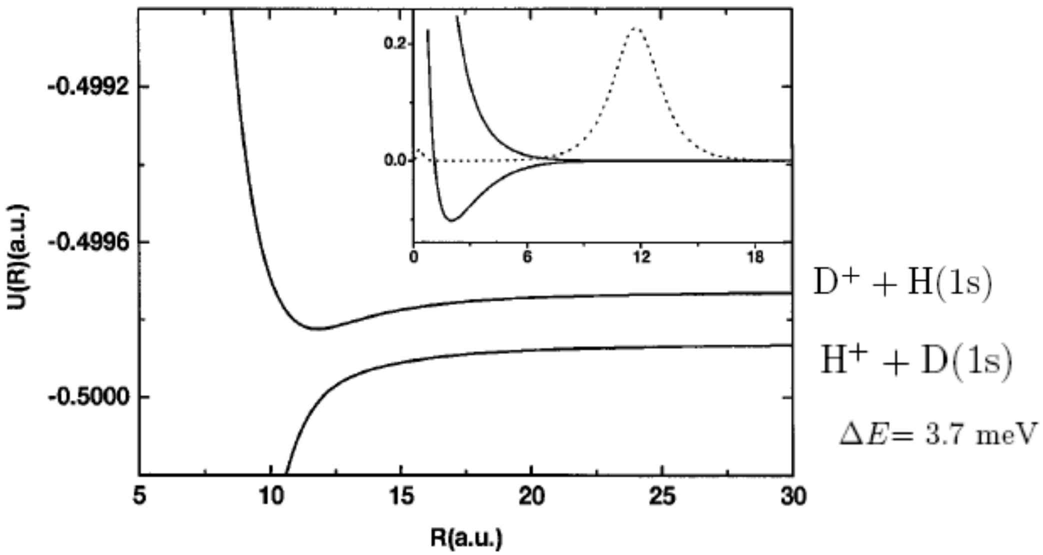


Resonances assosiated with $(p\mu)_{1s}$ threshold in $^3\mathrm{He}^{2+} + p\mu$ system.

Partial wave	(E_r , Γ) in eV
0	$(-73.70,\ 5.6[-3])^{HS}$
	$(-72.76,\ 6.4[-3])^{B}$
1	$(-41.73,\ 2.8[-3])^{HS}$
	$(-38.82,\ 3.1[-3])^{B}$
2	$(7.2\ ,\ 1.9)^{HS}$

^{B} Balyaev *et al.*

S-wave adiabatic potential curves of $D^{+} + H(1s)$ system



The lowest curve for $J = 0$ supports 23 bound states.

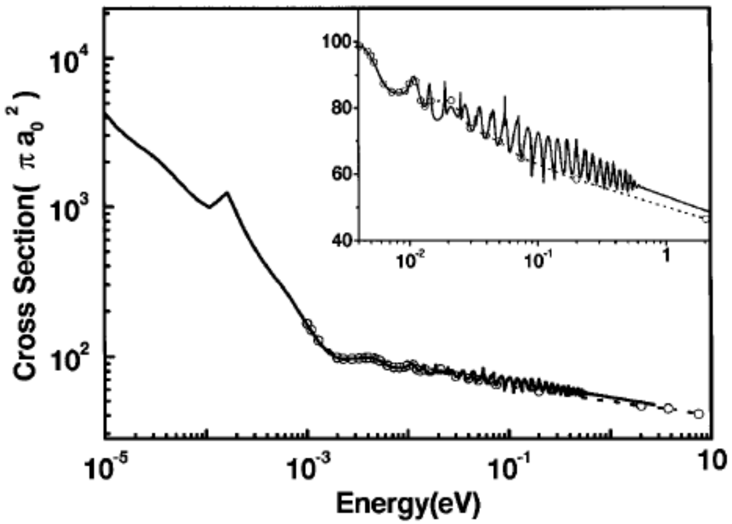
The lowest one: 2.67 eV

Energies and widths (in cm^{-1}) for resonances near H(1s) thershold.

	Energy	Width	Energy	Width[a]
$J = 0$	−5.827	4.26	−5.868	5.261
$J = 1$	−5.190	3.71	−5.196	4.632
$J = 2$	−3.839	2.79	−3.769	3.336
$J = 3$	−1.496	1.56	−1.478	1.707
$J = 4$	1.190	0.55		
$J = 5$	4.080	2.81		
$J = 6$	7.249	7.62		

[a] Wolniewicz *et al.*

Total cross section for $D^{+} + H(1s) \rightarrow D(1s) + H^{+}$



Summary

- HS approach for 3-body Coulomb systems are explained.
- In HS coordinates, the whole system Is described by (ρ, Ω), allowing the collective description of particles in the system.
- The whole wavefunction is expanded with the adiabatic channel function, in which the correlation among particles is considered.
- Inspection of potential curves is helpful to understand the dynamics of bound and resonance states.
- The single-channel approximation is already a fairly good approximation in many cases.
- When HS channels are coupled, the convergence is generally rapid due to the suitability for strongly correlated quantal systems.

- There are four-body treatment for three-electron atomic system (Li etc). The extension to general four-body Coulomb systems is desired.