Finite Size Correction to the ddμ and dtμ Molecules

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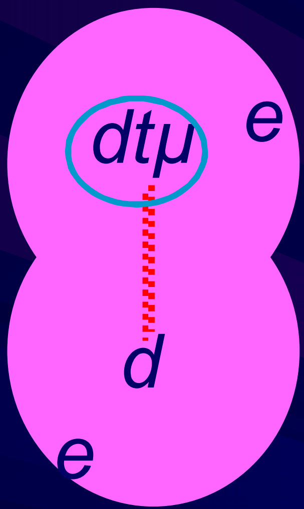
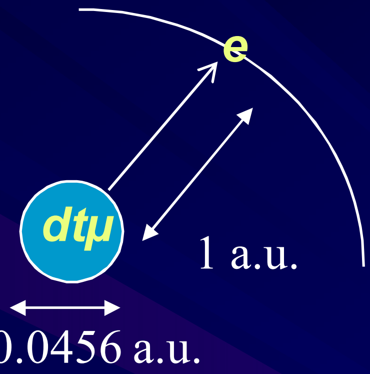
Finite Size Correction

6-body calculation



4-body calculation x 1.45



Scaled by density

$$\Delta E^{\mathrm{FS}} = E^{dt\mu e} - \varepsilon_{1s}^{(dt\mu)-e} - \varepsilon_{11}^{dt\mu} - \varepsilon_{1s}^{t\mu}$$

4-body calculation (1-st order , 2-nd order purterbation)

Harston, Hara, Kino, Shimamura, Sato, Kamimura

0.50 meV : $E^{(1)}+E^{(2)}=18.253-17.752 = 0.50$

1.46 meV : $E^{(1)}+E^{(2)}=11.577-10.113 = 1.46$

In the previous calculation,

1-st order $\approx$ 2-nd order

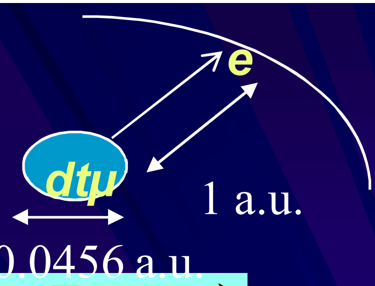
Purpose of this work :

to make full 4-body calculation

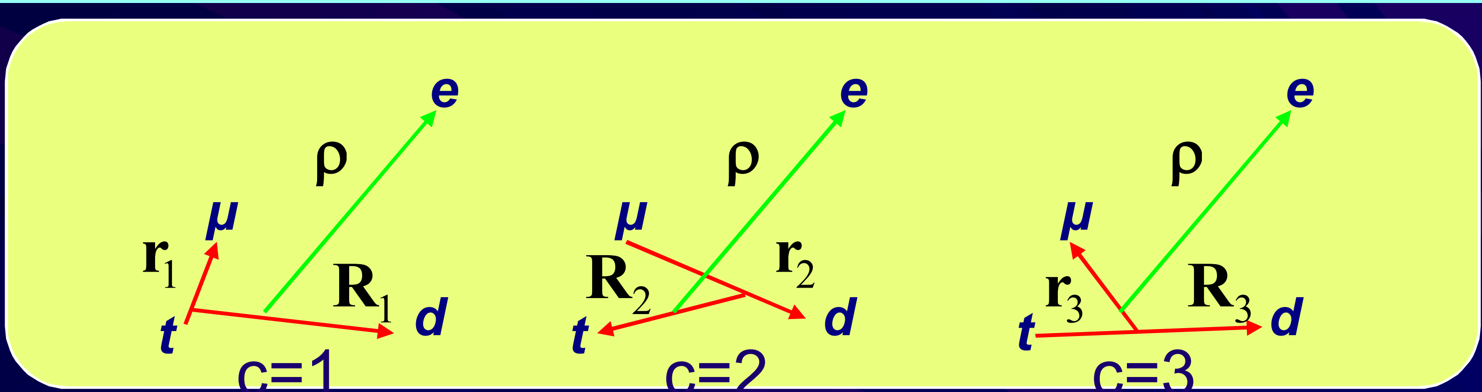
and see the higher-oder contribution

Gaussian Expansion Method (GEM)

E. Hiyama et al., Prog. Part. Nucl. Phys. **51**, 223, 2003



$$\Psi_{jwJM} = \Psi_1(\mathbf{r}_1,\mathbf{R}_1,\boldsymbol{\rho}) + \Psi_2(\mathbf{r}_2,\mathbf{R}_2,\boldsymbol{\rho}) + \Psi_3(\mathbf{r}_3,\mathbf{R}_3,\boldsymbol{\rho})$$



$$\Psi_c(\mathbf{r}_c,\mathbf{R}_c,\boldsymbol{\rho}) = \sum_{lL\lambda\Lambda} \sum_{aA\alpha} r_c^l R_c^L \rho^\Lambda \exp(-ar^2 - AR^2 - \alpha\rho^2)\left[\left[Y_l(\hat{\mathbf{r}}_c)\otimes Y_L(\hat{\mathbf{R}}_c)\right]_\lambda \otimes Y_\Lambda(\hat{\boldsymbol{\rho}})\right]_{JM}$$

Inner angular momentum coupling: $\vec{l} + \vec{L} = \vec{\lambda} \qquad \vec{\lambda} + \vec{\Lambda} = \vec{J}$

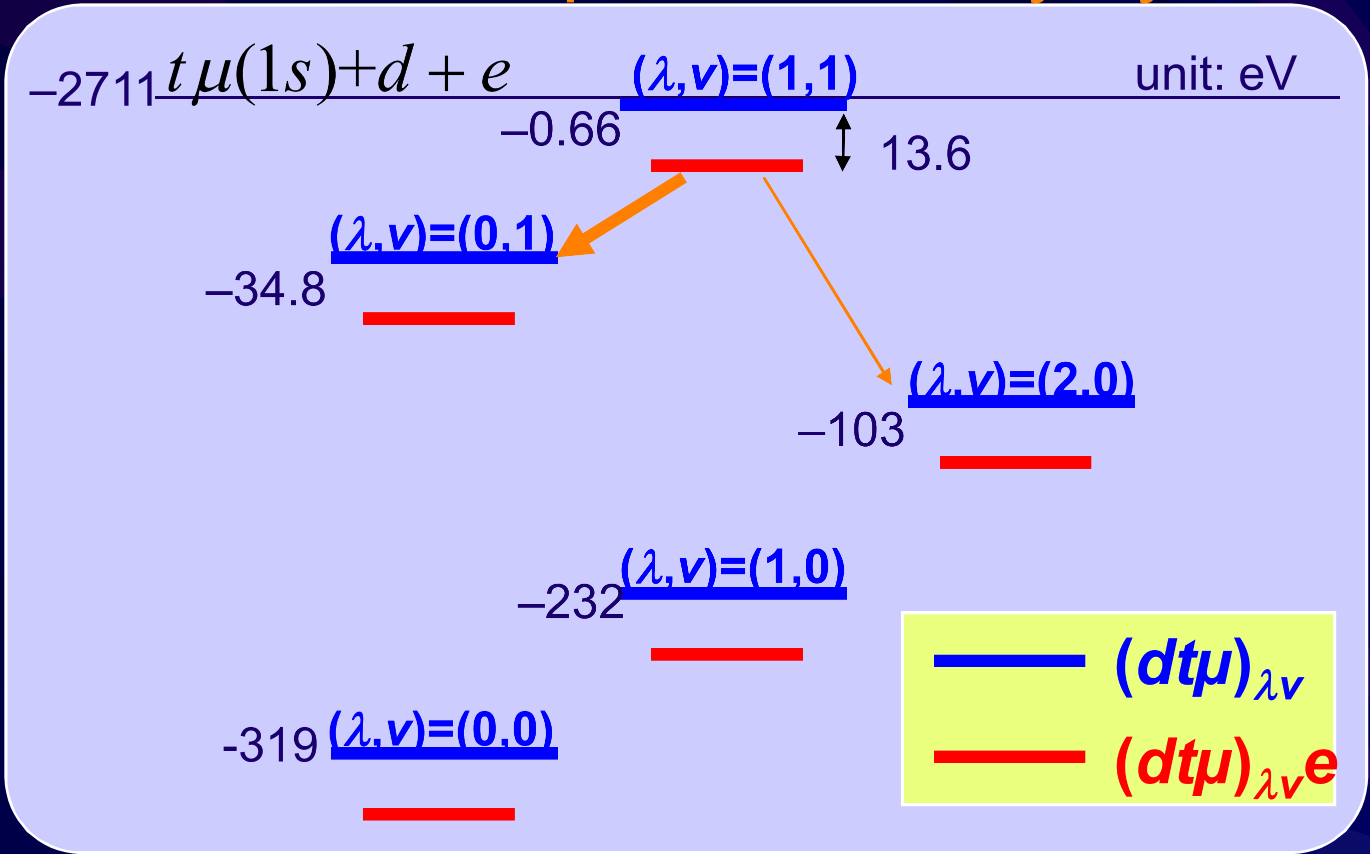
$$0 \le l \le 6 \qquad 0 \le L \le 6 \qquad 0 \le \lambda \le 3 \qquad 0 \le \Lambda \le 3$$

#(basis) ≤ 17 for 2-body H *atom*

#(basis) ≤ 3,100 for 3-body *dtμ*

#(basis) ≤ 180,000 for 4-body *dtμe*

dtμ-e four-body system

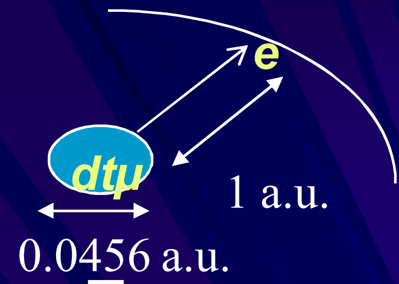


$(dt\mu)_{\lambda v}e$: Resonance state

$(dt\mu)_{\lambda v}e \rightarrow (dt\mu)_{\lambda' v'} + e$ Auger transition

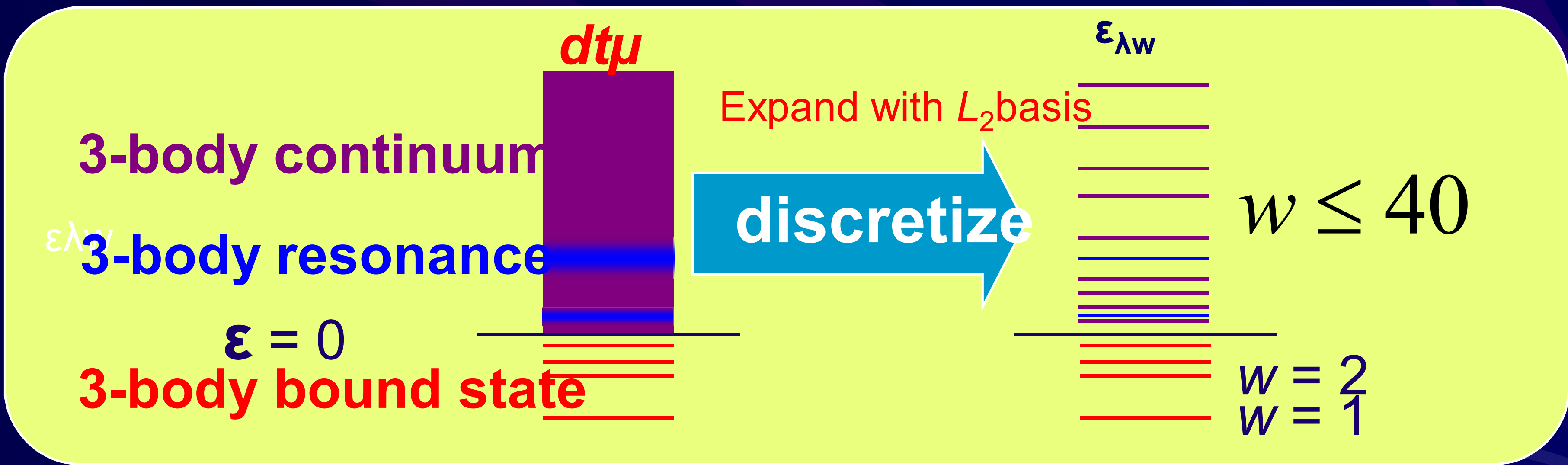
4-body wavefunction

$\Psi^{dt\mu e}_{jvJM}$



1st step: three-body, 2nd step: CC calculation for e

$$\Psi^{dt\mu e}_{jvJM} = \sum_{\Lambda}\sum_{\lambda w} C_{\lambda w}\left[\Phi^{dt\mu}_{\lambda w}\otimes f^{dt\mu-e_{jv}}_{\lambda\Lambda}(\rho)\right]_{JM}$$



Subsystem: 0.01 meV accuracy @ dtμ, ddμ, H

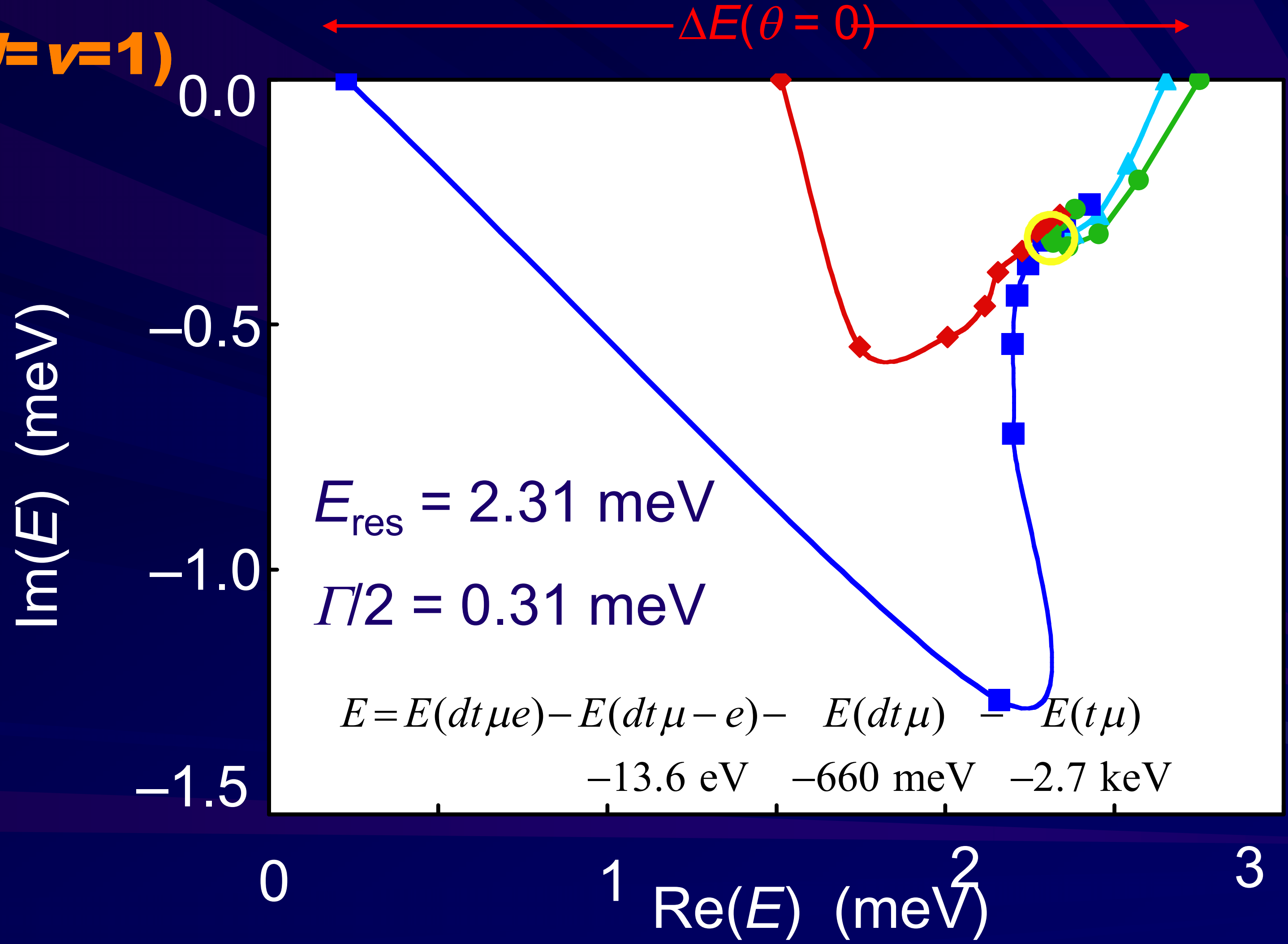
dtμ: Korobov, *J. Phys. B* ***37****, 2331, 2004*

Complex Coordinate Rotation method

$$r \to \alpha \exp(\mathrm{i}\theta) r,\ \ R \to \alpha \exp(\mathrm{i}\theta) R,\ \ \rho \to \alpha \exp(\mathrm{i}\theta)\rho$$

$$\left\langle \Phi_{vJM}(\theta) \middle| H(\theta) \middle| \Phi_{v'JM}(\theta) \right\rangle = E_{vJ}(\theta)\delta_{vv'}$$

dtμ(J=v=1)



The complex coordinate rotation method is absolutely necessary

Finite Size Correction **Full 4-body calculation**

$$\Delta E^{\mathrm{FS}} = E^{dt\mu e} - \varepsilon_{1s}^{(dt\mu)-e} - \varepsilon_{11}^{dt\mu} - \varepsilon_{1s}^{t\mu}$$

previous

4-body calculation (1-st order , 2-nd order purterbation)

Harston, Hara, Kino, Shimamura, Sato, Kamimura

dtμ 0.50 meV : $E^{(1)} + E^{(2)} = 18.253 - 17.752 = 0.50$

ddμ 1.46 meV : $E^{(1)} + E^{(2)} = 11.577 - 10.113 = 1.46$

This work

dtμ 2.31 meV

ddμ 1.70 meV

correction (dtμ) .> correction (ddμ)

size (dtμ) > size (ddμ)

reasonable

Concluding remark

1) we, for the first time, calculate the full four-body dtmu-e system and obtained the finite size correction, and found that the previous second-order purterbation calculation was not a good approximation.

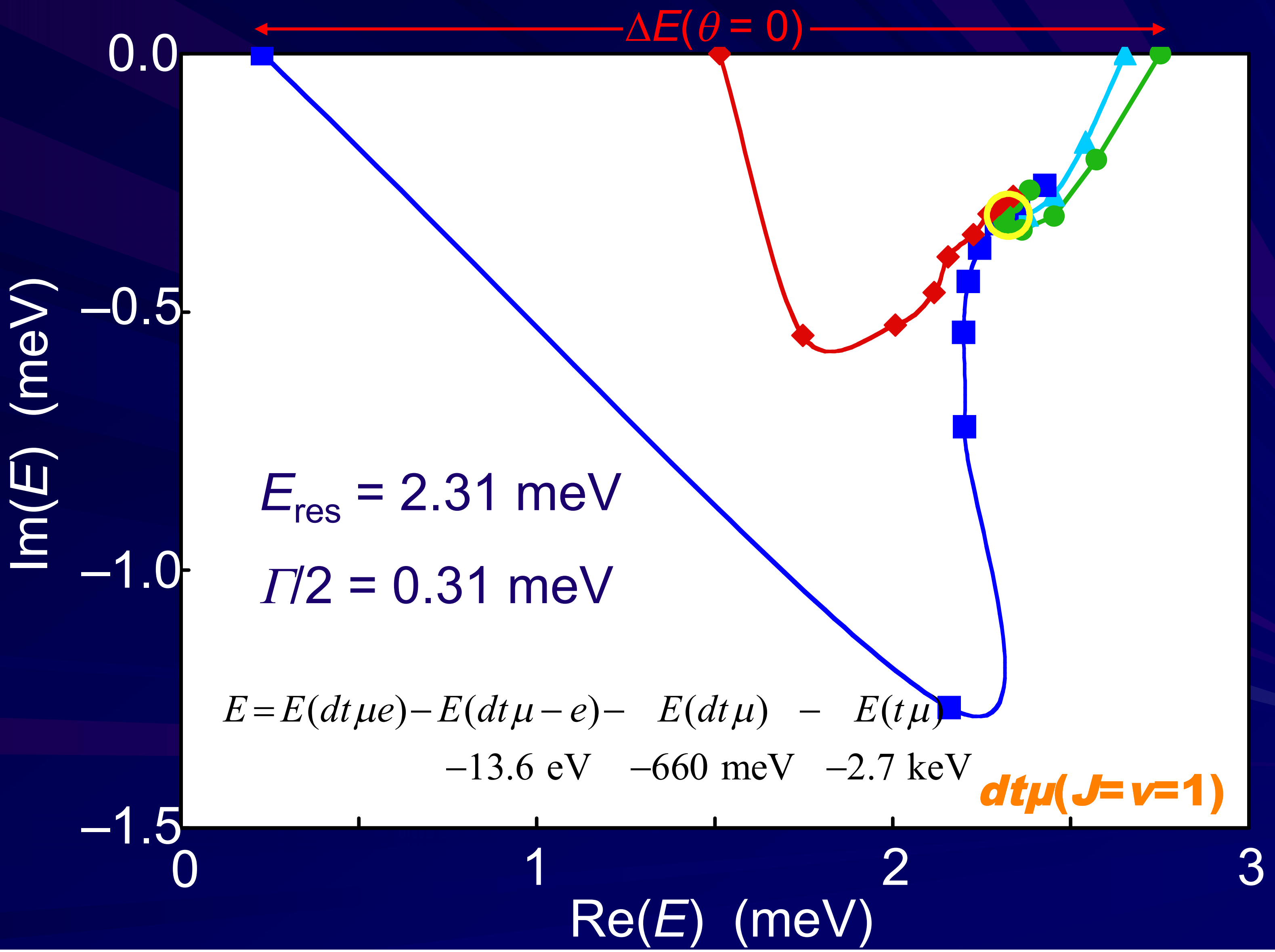
2) The four-body systems are not true bound states but resonance states. Use of the complex coordinate rotation method is absolutely necessary since the accuracy of the calculation without complex coordinate rotation is worse than the required accuracy.

3) These consideration will be necessary in the six-body calculation of the correction.

Complex Coordinate Rotation method

$$r \to \alpha \exp(\mathrm{i}\theta) r, \quad R \to \alpha \exp(\mathrm{i}\theta) R, \quad \rho \to \alpha \exp(\mathrm{i}\theta)\rho$$

$$\left\langle \Phi_{vJM}(\theta) \middle| H(\theta) \middle| \Phi_{v'JM}(\theta) \right\rangle = E_{vJ}(\theta)\delta_{vv'}$$



Finite size correction

$$\Delta E^{\mathrm{FS}} = E^{dt\mu e} - \varepsilon_{11}^{dt\mu} - \varepsilon_{1s}^{(dt\mu)-e}$$

Authors	ΔE^{FS} **(meV)**	Syste
Harston, Hara, Kino, Shimamura, Kamimura	0.50 ($E^{(1)}+E^{(2)}$=18.253–17.752) 1.46 ($E^{(1)}+E^{(2)}$=11.577–10.113)	($dt\mu$) ($dd\mu$
This Work	0.25 **2.31** 0.30 **1.70**	($dt\mu$ **($dt\mu$** ($dd\mu$ **($dd\mu$**

Summary

- Energy levels and widths of 4-body resonance states ***dtμe***、***ddμe*** are calculated with the use of the Gaussian expansion method and the complex coordinate rotation method.

- The results significantly differ from the literature values calculated by the 2nd order perturebation).

dtμe Resonance effect is important

$\Delta E(\theta=0) \sim \mathrm{Re}(E)$.

Auger decay rate $2.5\times10^{12}\ \mathrm{s}^{-1}$

ddμe ***Full-finite size correction:***

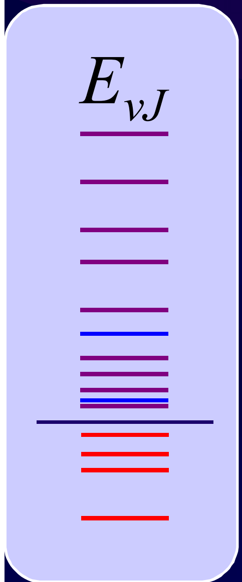
$\varepsilon_{11}(dd\mu)$ –1964.83 meV Theory (2nd perturbation)

–1963.83 meV Theory (this work: scaling)

–1962.6(3) meV Experiment

Contribution from bound states and *pseudo* states of dtμ molecle**dtμ(J=1, v=0)**

$$\Psi^{dt\mu e}_{jvJM} = \sum_{\Lambda}\sum_{\lambda w} C_{\lambda w}\left[\Phi^{dt\mu}_{\lambda w} \otimes f^{dt\mu - e}_{jv,\Lambda}(\rho)\right]_{JM} \qquad \left|\left\langle \Phi^{dt\mu}_{v\lambda} \middle| \Psi^{dt\mu e} \right\rangle\right|^2$$



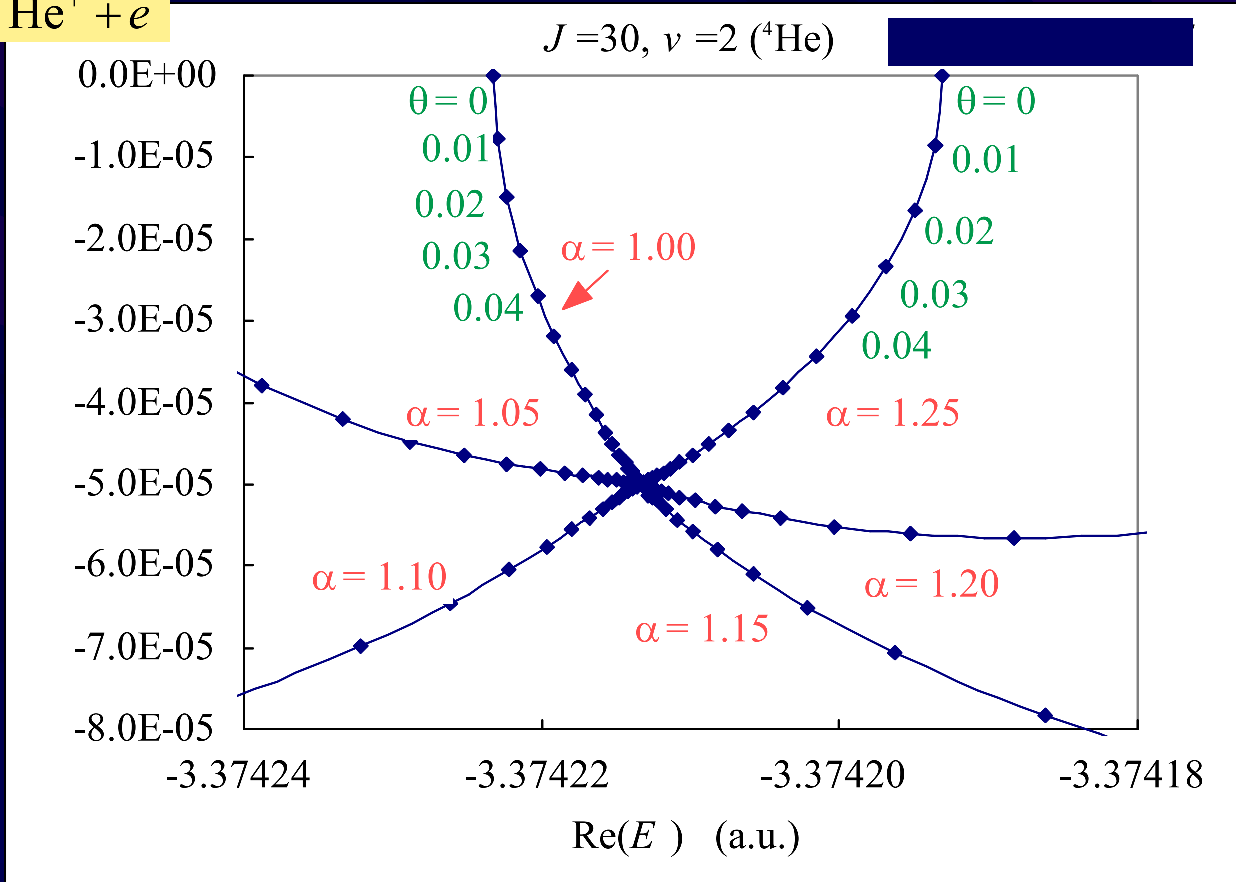
v	*λ*	*Λ*	*dtμ*(10)	*dtμ*(11)	*ddμ*(10)	*ddμ*(11)
0 (–200 eV)	1	0	0.9999995677		0.9999998333	
1 (–1 eV)	1	0		0.9996957732		0.9998987096
E>0	1	0		0.0000769941		0.0000032048
0 (–300 eV)	0	1	0.0000002449			
1 (–30 eV)	0	1		0.0000252470		
E>0	0	1	0.0000000109	0.0000791740	0.0000000377	0.0000400018
0 (–100 eV)	2	1	0.0000000530	0.0000007447		
E>0	2	1	0.0000000385	0.0001218511	0.0000000868	0.0000579452
0 (–200 eV)	1	2				
1 (–1 eV)	1	2		0.0000000392		0.000000017

複素座標回転法相対論補正(Darwin ter

$r \to \alpha \exp(\mathrm{i}\theta) r \quad R \to \alpha \exp(\mathrm{i}\theta) R$

$$\langle \Phi_{vJM}(\theta) | H(\theta) | \Phi_{v'JM}(\theta) \rangle = E_{vJ}(\theta) \delta_{vv'}$$

$\overline{p}\mathrm{He}^+ = \overline{p} + \mathrm{He}^+ + e^-$



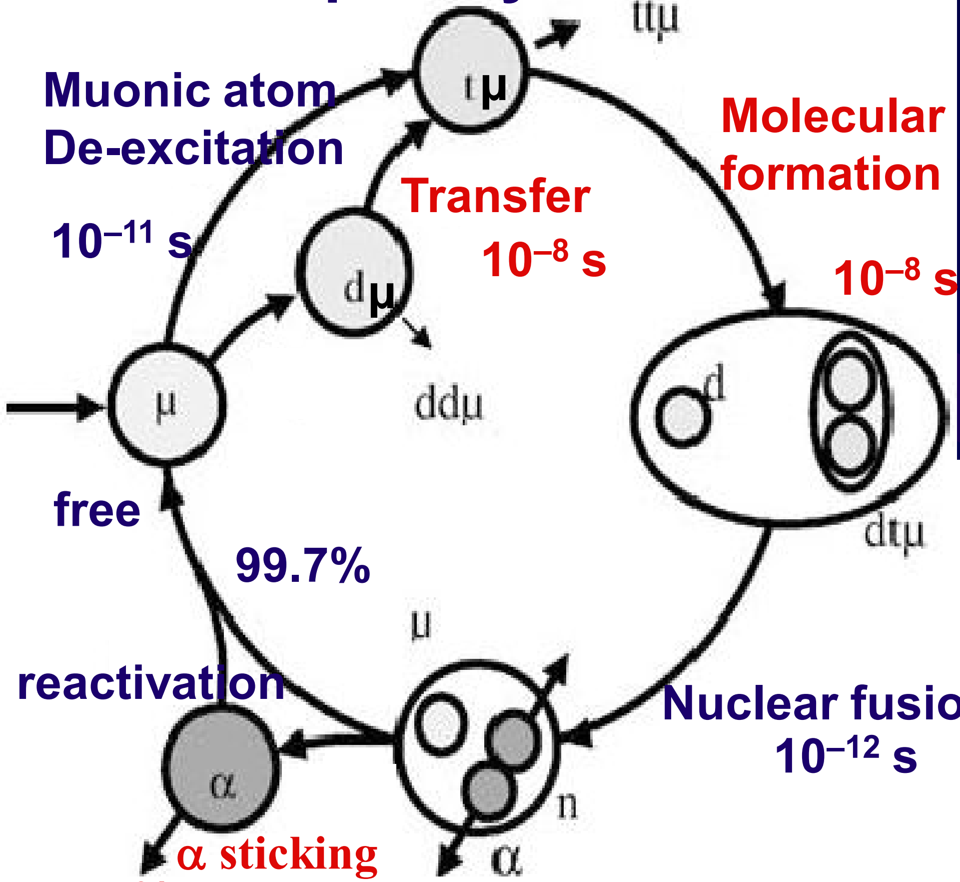
Complex eigenenergy trajectories

$(E_r, -\Gamma/2) = (-3.374\ 213\ 517,\ 0.000\ 049\ 331)$

分光実験値と高精度で一致（反陽子の質量を10 ppb (10^{-8})の精度で決定）

muon catalyzed fusion (μCF)

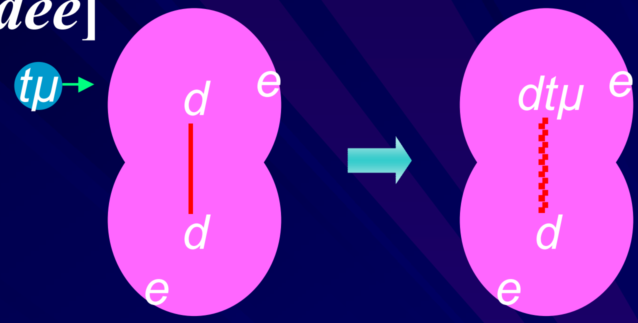
μCF cycle



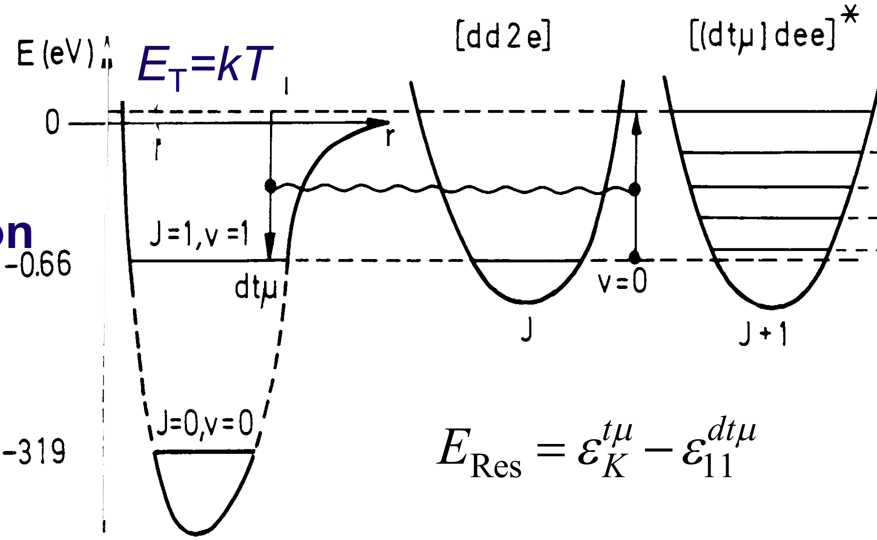
dtμ □ *α*+*n*+*μ*+17.6 MeV

Complex molecular formation

[(*dtμ*)*dee*]



Resonant reaction



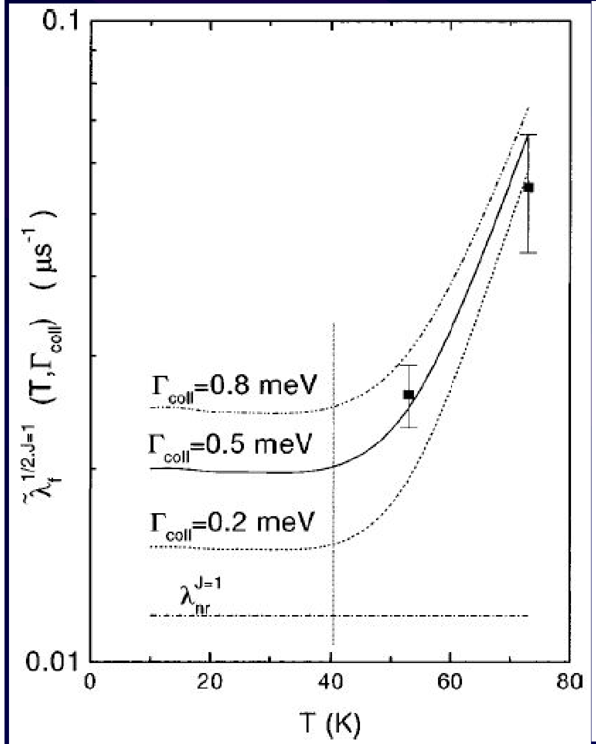
$$E_{\mathrm{Res}} = \varepsilon_K^{t\mu} - \varepsilon_{11}^{dt\mu}$$

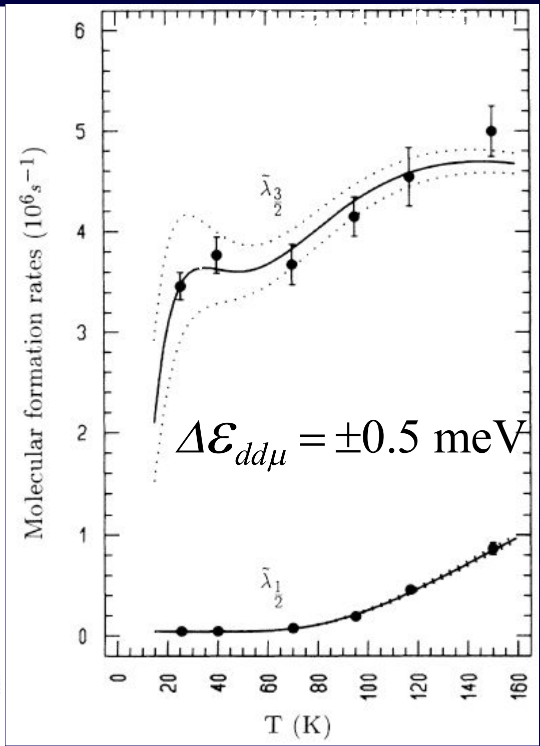
150 cycles/μ⁻ (at present)

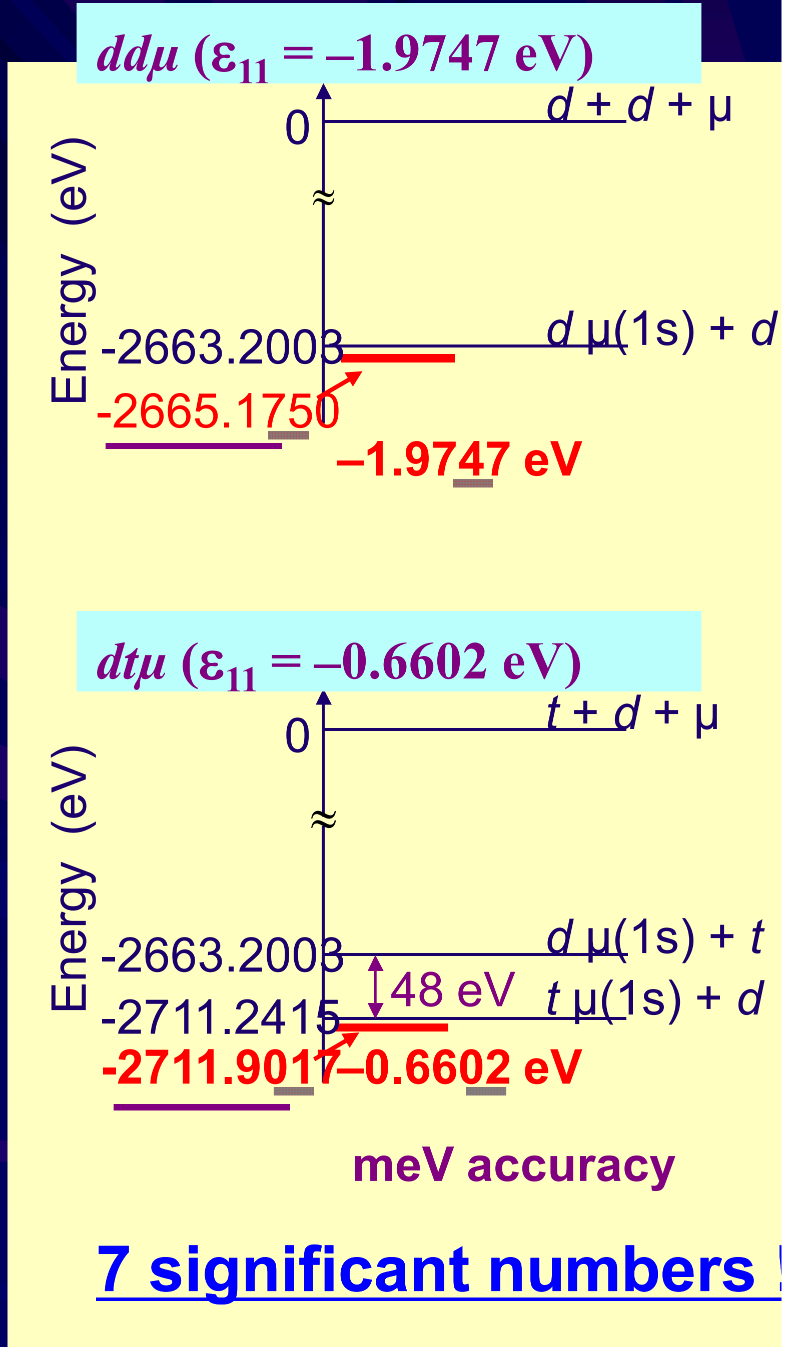
300 cycles/μ⁻ (input)=(output)

$$E(dt\mu) + E_T = E_{Jv}([(dt\mu)d\ ee]^*)$$

Sub-meV accuracy in three-body calculation is required

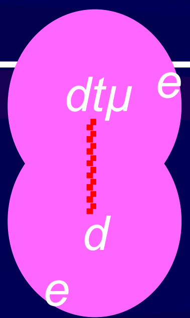


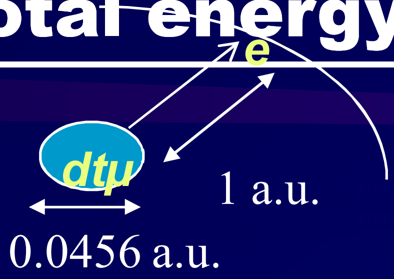




Relativistic and other corrections (meV)

	ddμ	dtμ
Vacuum polarization	8.720	16.617
Electromagnetic structure	–1.675	13.183
Relativistic shift	1.650	0.853
Full finite size	1.46	0.50
Nuclear polarization	0.0	–1.7
Total shift	10.16	29.4
Non-relativistic energy	–1974.985	–660.336
Total energy	–1964.83	–630.9





Full finite size (six-body)
Finite size (four-body)

Finite size correction

$$\Delta E^{\mathrm{FS}} = E^{dt\mu e} - \varepsilon_{1s}^{(dt\mu)-e} - \varepsilon_{11}^{dt\mu} - \varepsilon_{1s}^{t\mu}$$

Authors	ΔE^{FS} **(meV)**	System
Menshikov	8	$(dt\mu)_{11}e$
Bakalov	1.2	$(dt\mu)_{11}e$
Scriniz, Szalewicz	$0.2_{-0.1}^{+0.2}$, 0.54	$(dt\mu)_{11}e$
Harston, Kamimura, Shimamura	0.58, 0.50	$(dt\mu)_{11}e$
Harston, Hara, Kino, Shimamura, Sato, Kamimura	**90.40** ($E^{(1)}+E^{(2)}$=18.253–17.850) **1.45** ($E^{(1)}+E^{(2)}$=11.577–10.12)	$(dt\mu)_{11}e$ $(dd\mu)_{11}e$

Finite size correction

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This Work	? ?	$(dt\mu)_{11}e$ $(dd\mu)_{11}e$

Finite size correction

Harston, Hara, Kino, Shimamura, Sato, Kamimura

0.40 meV $E^{(1)}+E^{(2)}=18.253-17.752 = 0.50$

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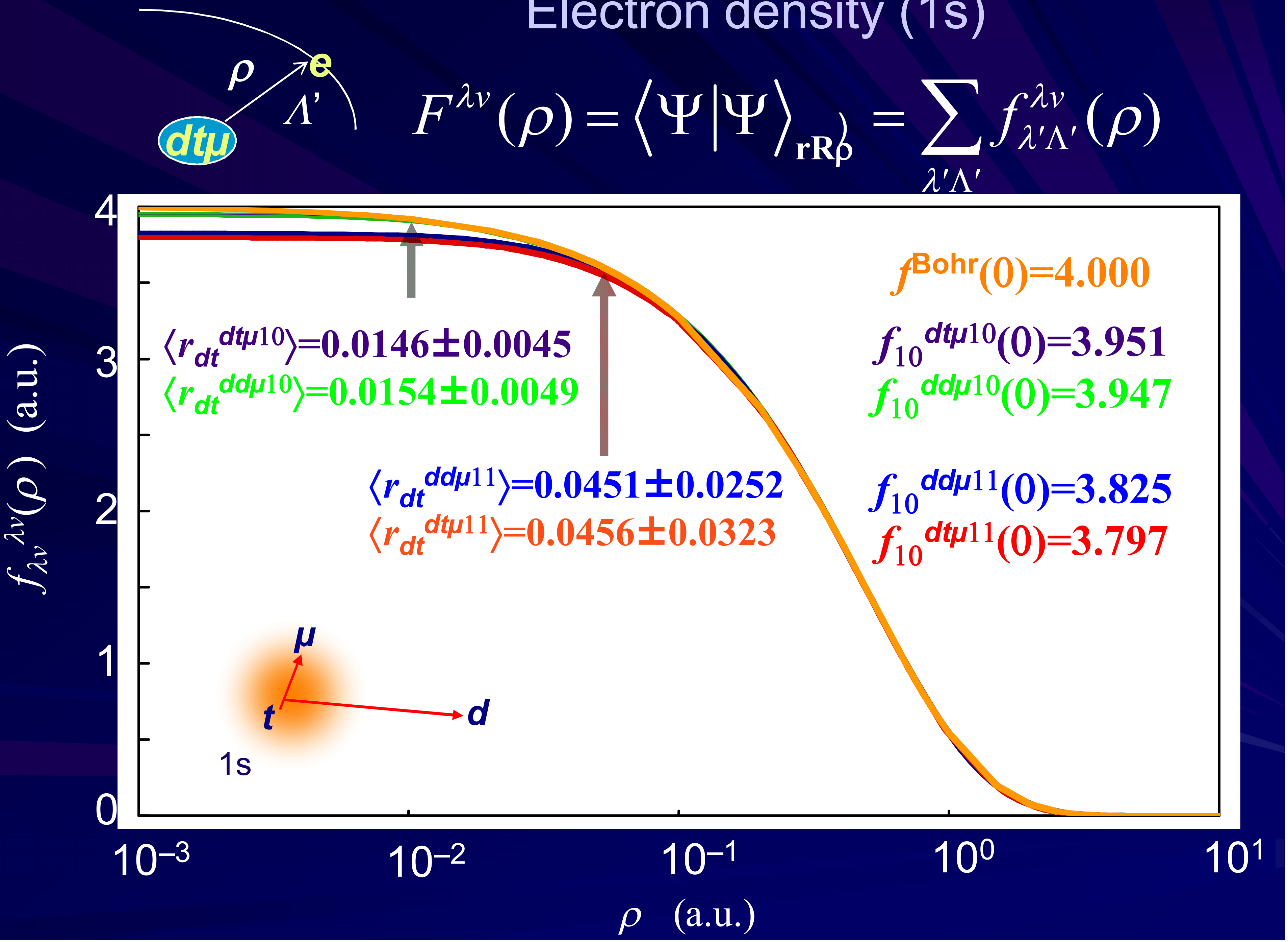
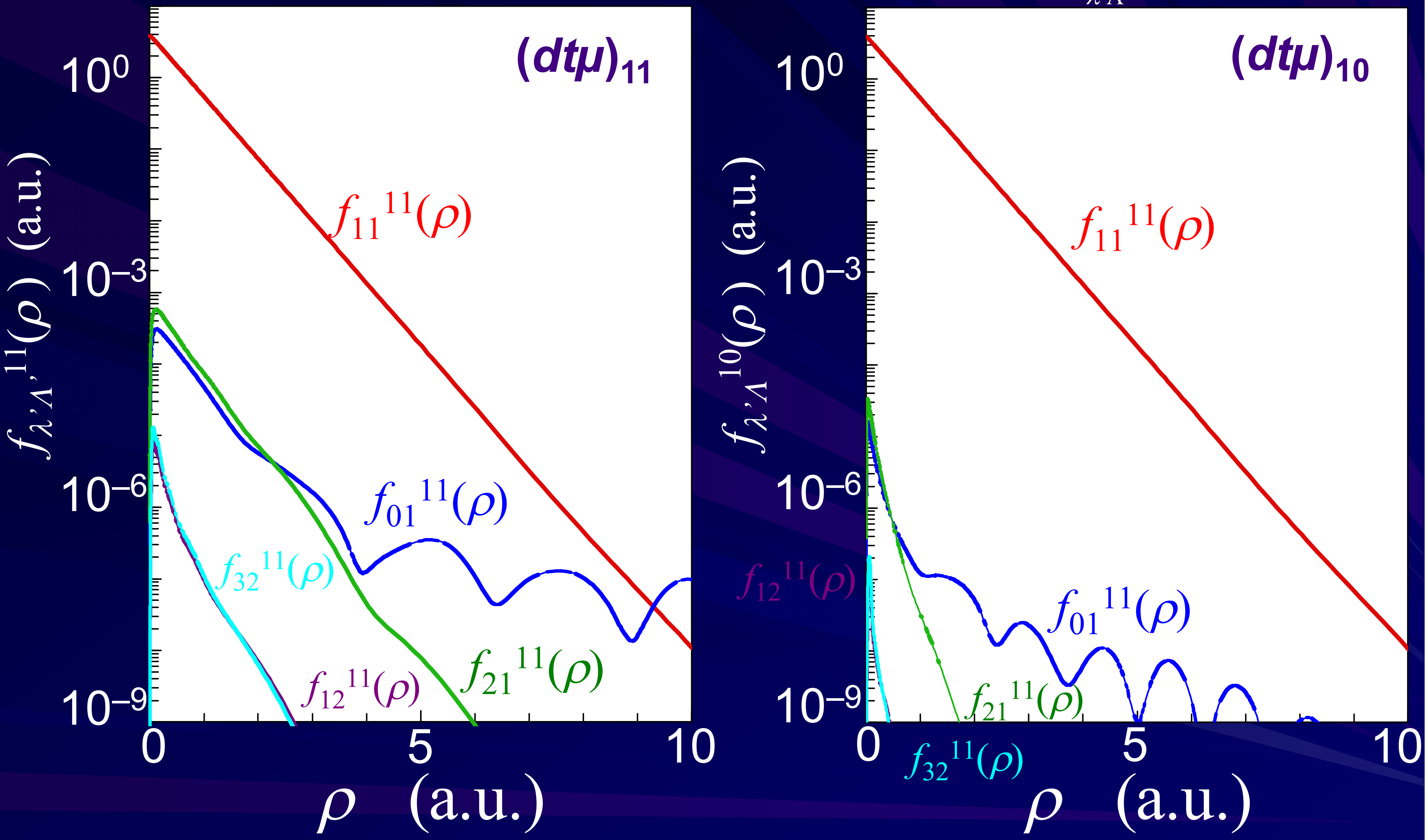
Electron density (1s)

$$F^{\lambda v}(\rho) = \langle \Psi | \Psi \rangle_{\mathrm{rR}\rho} = \sum_{\lambda'\Lambda'} f^{\lambda v}_{\lambda'\Lambda'}(\rho)$$



Electron densities

$$F^{\lambda v}(\rho) = \langle \Psi | \Psi \rangle_{\mathbf{rR}\hat{\rho}} = \sum_{\lambda'\Lambda'} f^{\lambda v}_{\lambda'\Lambda'}(\rho)$$



$$\lim_{\rho\to\infty} f^{\lambda v}_{\lambda' v'}(\rho) = \mathrm{e}^{\mathrm{i}(\kappa - \mathrm{i}\gamma)\rho} \xrightarrow[\rho \to e^{\mathrm{i}\theta}\rho]{} \mathrm{e}^{\mathrm{i}(\kappa-\mathrm{i}\gamma)\rho(\cos\theta + \mathrm{i}\sin\theta)} = e^{-(\kappa\sin\theta - \gamma\cos\theta)\rho + \mathrm{i}(\kappa\cos\theta + \gamma\sin\theta)\rho}$$