本征通道R-矩阵的进展

为相关学科领域提供原子物理参数的一种方案

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Outline

1. 谈谈需求的背景
   多！ 精确！

2. 介绍一种“完美原子物理方案”，可以为为相关学科领域提供原子物理参数。
   希望以具体例子向大家阐明，为什么我们提出的方案是“完美”的？
   着重阐明理论方法的物理图像。

3. 总结讨论

需求的背景

- **fusion energy researches, astrophysics, space sciences, …**

  To simulate numerically temporal-spatial motions of plasmas and to perform diagnostic analysis about plasma's conditions: atomic energy levels and related collision processes…

  Present requirements: not only enormous but also accurate enough

  Therefore to compile such atomic data can not be finished completely by experimental measurements.

- **Theoretical computations should play indispensable role to satisfy needs.**

等离子体中的原子物理； 对于未完全离化原子过程；
量子多体理论 !!!!!!!! 本次汇报的重点 !!!!!!!!

在激光聚变过程涉及能量输运、能量耗损、甚至宏观内爆过程

电子-原子过程

$$e + A(\text{包括原子离子}) \leftrightarrow e + A$$

$$e + A \leftrightarrow e + A^{*}; \qquad A^{*} \rightarrow A + h\nu$$

$$e + A^{*} \leftrightarrow e + A^{**}; \qquad A^{**} \rightarrow A^{*} + h\nu$$

$$e + A \leftrightarrow e + e + A^{*}$$

$$e + A^{*} \leftrightarrow e + e + A^{**}$$

$$e + A \leftrightarrow e + A + h\nu$$

光子-原子过程

$$h\nu + A \leftrightarrow A^{*}$$

$$h\nu + A^{*} \leftrightarrow A^{**}$$

$$h\nu + A \leftrightarrow A^{+*} + e$$

$$h\nu + A^{*} \leftrightarrow A^{+**} + e$$

$$h\nu + A \leftrightarrow A^{**} \leftrightarrow A^{+*} + e$$

$$h\nu + A^{*} \leftrightarrow A^{**} \leftrightarrow A^{+*} + e$$

“多、快、好、省”

物理精密化要求！

物理模拟

诊断分析

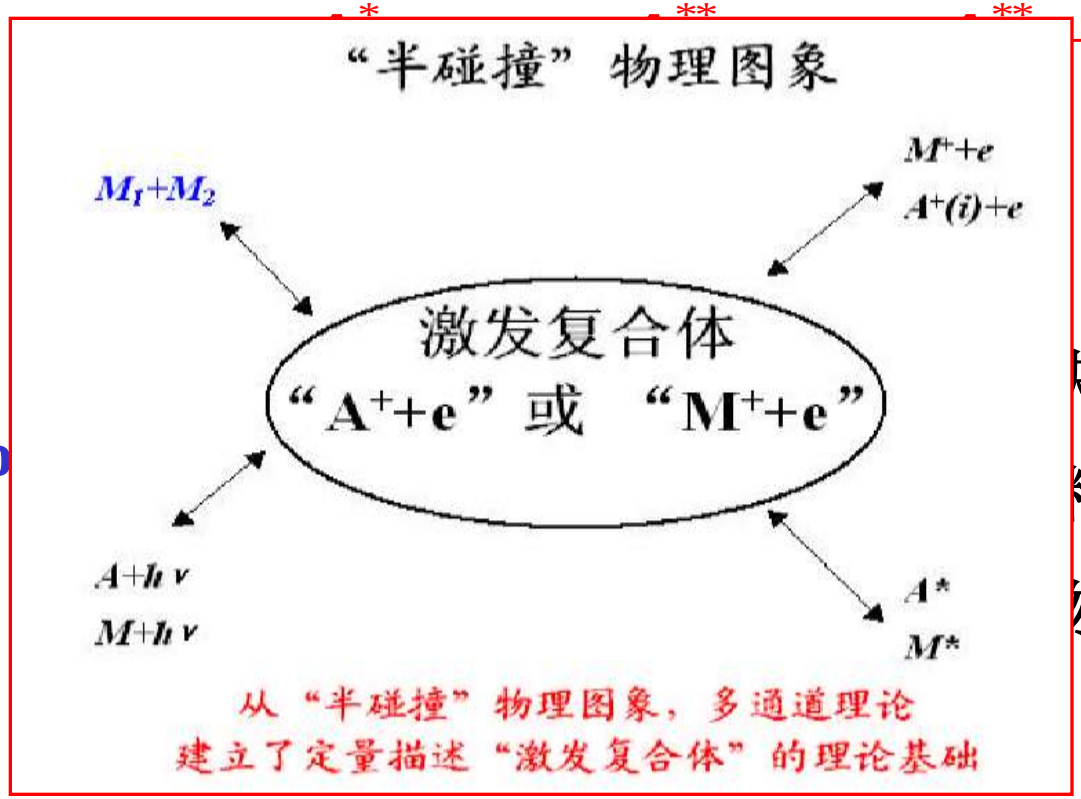
“完美原子物理方案”

electron-atom/ion

$$e + A(\text{包括原子离子}) \leftrightarrow e + A$$

$$e + A \leftrightarrow e + A^{*}; \qquad A^{*} \rightarrow A + h\nu$$

$$\rightarrow A^{*} + h\nu$$



photon-atom/io

快、好、省”

精密化要求！

物理模拟

诊断分析

$$h\nu + A \leftrightarrow A^{**} \leftrightarrow A^{+*} + e$$

$$h\nu + A^{*} \leftrightarrow A^{**} \leftrightarrow A^{+*} + e$$

First, let me explain physical pictures of our theoretical computation methods

For Atomic Systems (including atomic ions) A^{+q}

most structures <------> dynamical processes

($A^{+(q+1)}$ + an electron)

Bound states **Continuum states**

↕ **(electron scattering processes)**

analytic continuation ⟷ scattering matrix

$$S_{ij} = \sum_{\alpha} U_{i\alpha} \exp\left(i\, 2\pi\mu_{\alpha}\right) U_{j\alpha}$$

It can be calculated by R-Matrix type methods.

R-Eigen Theoretical Method 最新进展

Brief introduction of R-Eigen Theoretical Method

(R-Eigen code)

Within the reaction zone, the interactions between the colliding electron and the target electrons involve electron exchange and correlation interactions. It is a many-electron problem, which can be solved variationally as a whole to obtain the logarithmic derivative boundary matrix R(E). [靶原子 + 电子]

Outside the reaction zone, the eigen-channel wavefunctions with normalization per unit energy can be expressed rigorously as,

$$\psi_\alpha = \sum_i U_{i\alpha} \cdot \Phi_i = \sum_i \phi_i \cdot U_{i\alpha} \cdot (f_i \cos \pi\mu_\alpha - g_i \sin \pi\mu_\alpha)$$

In the i^{th} physical ionization channel, *f* and *g* are regular and irregular Coulombic wave functions, respectively, which are continuous functions of the orbital energy across the ionization threshold, i.e., from the negative region to the positive region.

Cover all excited energy structure and electron-ion scattering processes !

In eigenchannel representation, scattering matrix is diagonalized, i.e., $S_{ij}^{J^\pi} = \sum_{\alpha}^{N} U_{i\alpha} \exp\left(i\, 2\pi\mu_\alpha\right) U_{j\alpha}$

N **eigen phase shifts** $\pi\mu_\alpha$, $N \times N$ **transformation matrix** $U_{j\alpha}$

and corresponding eigenchannel wavefunctions ψ_α

$$\psi_\alpha = \sum_i U_{i\alpha} \cdot \Phi_i = \sum_i \phi_i \cdot U_{i\alpha} \cdot (f_i \cos\pi\mu_\alpha - g_i \sin\pi\mu_\alpha)$$

are calculted by R-Eigen theoretical methods. The related transition matrix elements can also be calculted,

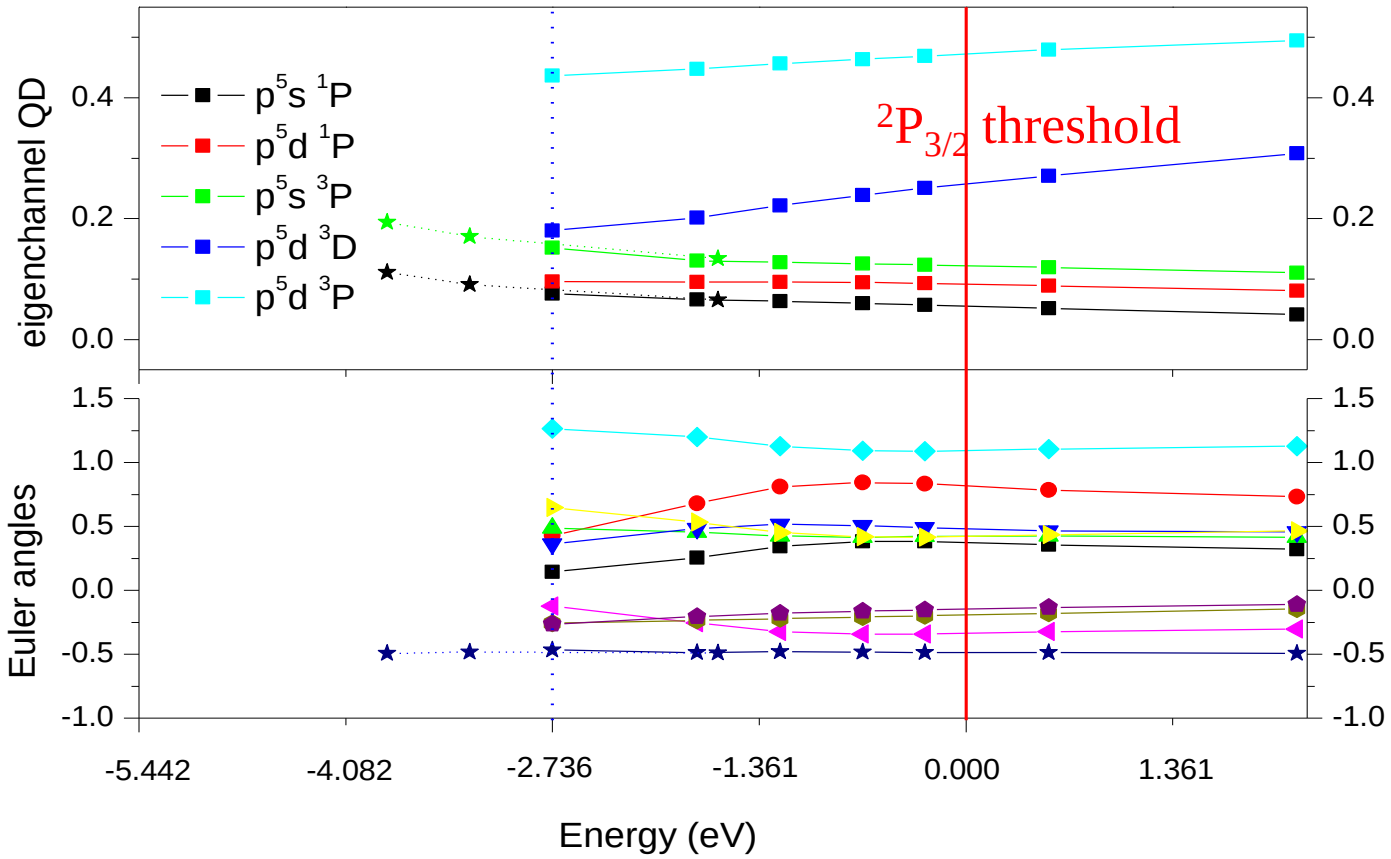
Note that $\pi\mu_\alpha$, $U_{j\alpha}$, ψ_α **and the related transition matrix elements (OS, GOS) are smooth functions of energy.**

“多、快、好、省”提供相关原子参数!

!!!! Analytical properties of scattering matrix !!!!

J.M. Li, X. Gao, et al., Plasma Science and Technology, 12, 335(2010).

Multi-Channel Example: $e + Kr^+ \longleftrightarrow Kr^*$



$e + Kr^+(^2P_{3/2,1/2})$; $J^\pi = 1^-$; $S_{ij}(5\times5)$; $5\,\mu_\alpha$, $U_{i\alpha}(5\times5) \Leftrightarrow 10\,\theta_{i\alpha}$

$J^\pi = 1^-$; 3 *channels* $Kr^+(^2P_{3/2}) + e(s_{1/2}, d_{5/2}, d_{3/2})$

2 *channels* $Kr^+(^2P_{1/2}) + e(s_{1/2}, d_{3/2})$

当应用 R-Eigen 理论方法，计算得到

$$\mu_\alpha \qquad U_{i\alpha}(N\times N) \leftrightarrow \theta_m\left(\frac{N\times(N-1)}{2}\right) \qquad \psi_\alpha$$

就能“准解析地”得到所有激发能级，以及相应碰撞过程的截面与速率。

在具体解释如何“准解析地”得到原子物理量以前，对确保计算精确作一些补充说明！

靶 + 电子

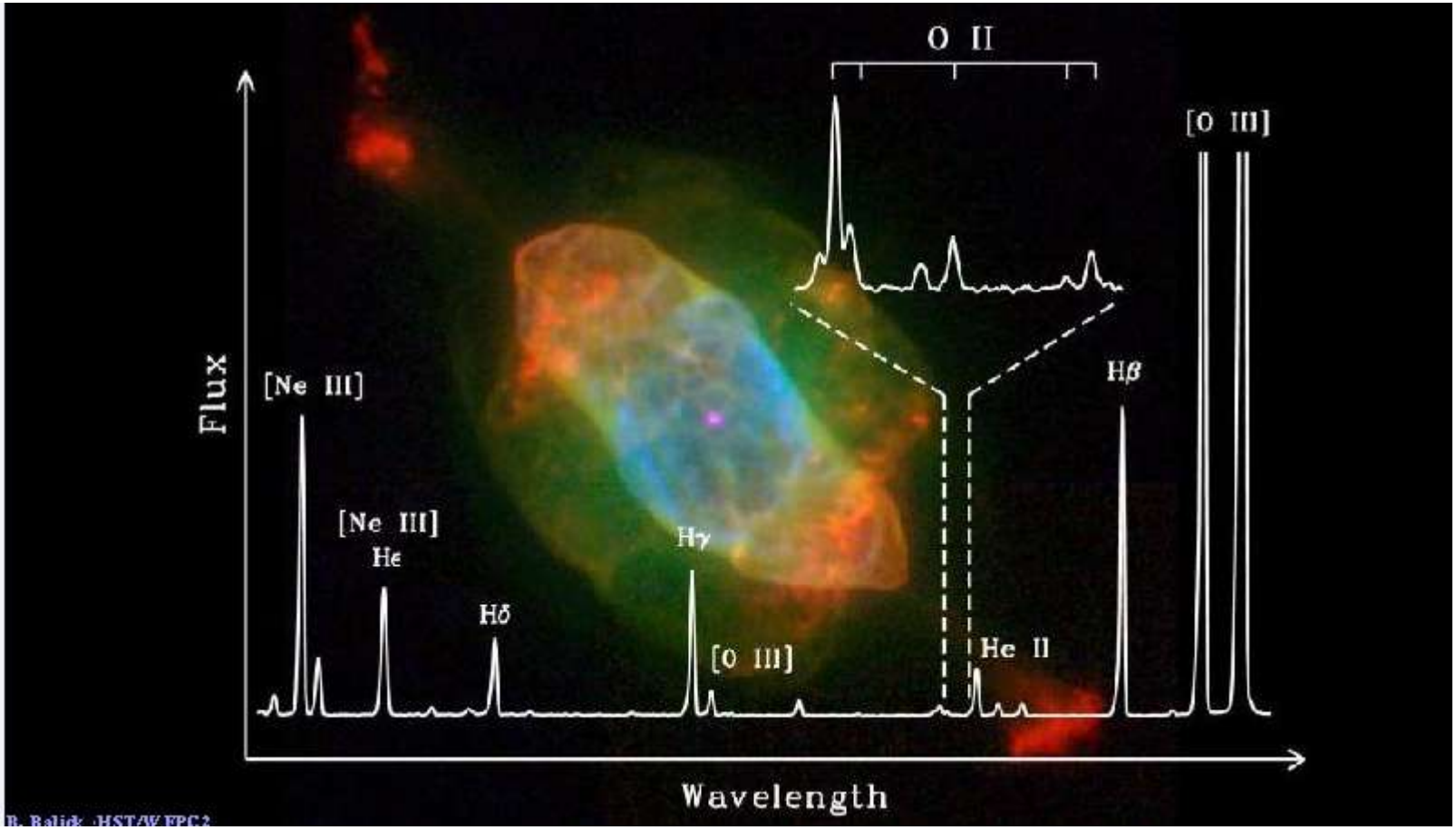
必须采用精确的靶态波函数!

例如，O^+ 来阐明如何得到精确的靶波函数

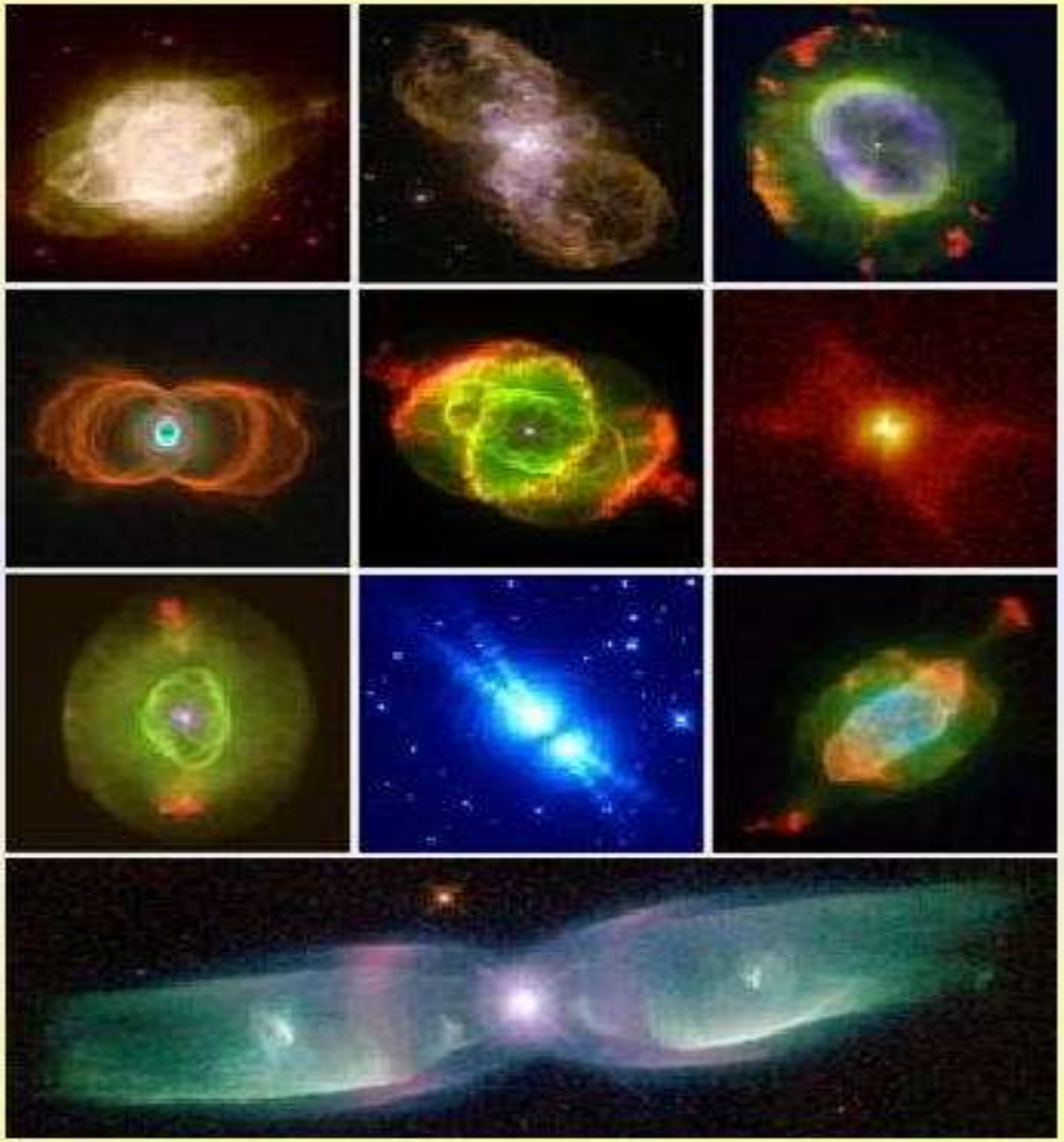
Benchmark forbidden transition rate ratio of OII ground state

$1s^2 2s^2 2p^3$ ($^4S_{3/2}$, $^2D_{5/2}$, $^2D_{3/2}$, $^2P_{3/2}$, $^2P_{1/2}$)

Also some interesting differences of transition rates between the fine structure levels


O II
[O III]
Flux
[Ne III]
[Ne III]
He
Hδ
Hγ
[O III]
He II
Hβ
Wavelength
B. Balick, HST/WFPC2

Ionized nebulae observed by ground telescope



B. Balick

0: ground state $^4S^o_{3/2}$

6: excited state $^2D^o_{5/2}$ $I_6 = N_6 A_6$

4: excited state $^2D^o_{3/2}$ $I_4 = N_4 A_4$

Rate equation：

$$\frac{dN_6}{dt} = \langle v\sigma_6 \rangle N_e N_0 - \langle v\sigma_{64} \rangle N_e N_6 + \langle v\sigma_{46} \rangle N_e N_4 - A_6 N_6 = 0$$

$$\frac{dN_4}{dt} = \langle v\sigma_4 \rangle N_e N_0 - \langle v\sigma_{46} \rangle N_e N_4 + \langle v\sigma_{64} \rangle N_e N_6 - A_4 N_4 = 0$$

$$N_6 = \frac{N_e^2 N_0 \langle v\sigma_{46} \rangle \left(\langle v\sigma_6 \rangle + \langle v\sigma_4 \rangle \right) + N_e N_0 \langle v\sigma_6 \rangle A_4}{N_e \left(\langle v\sigma_{46} \rangle A_6 + \langle v\sigma_{64} \rangle A_4 \right) + A_6 A_4}$$

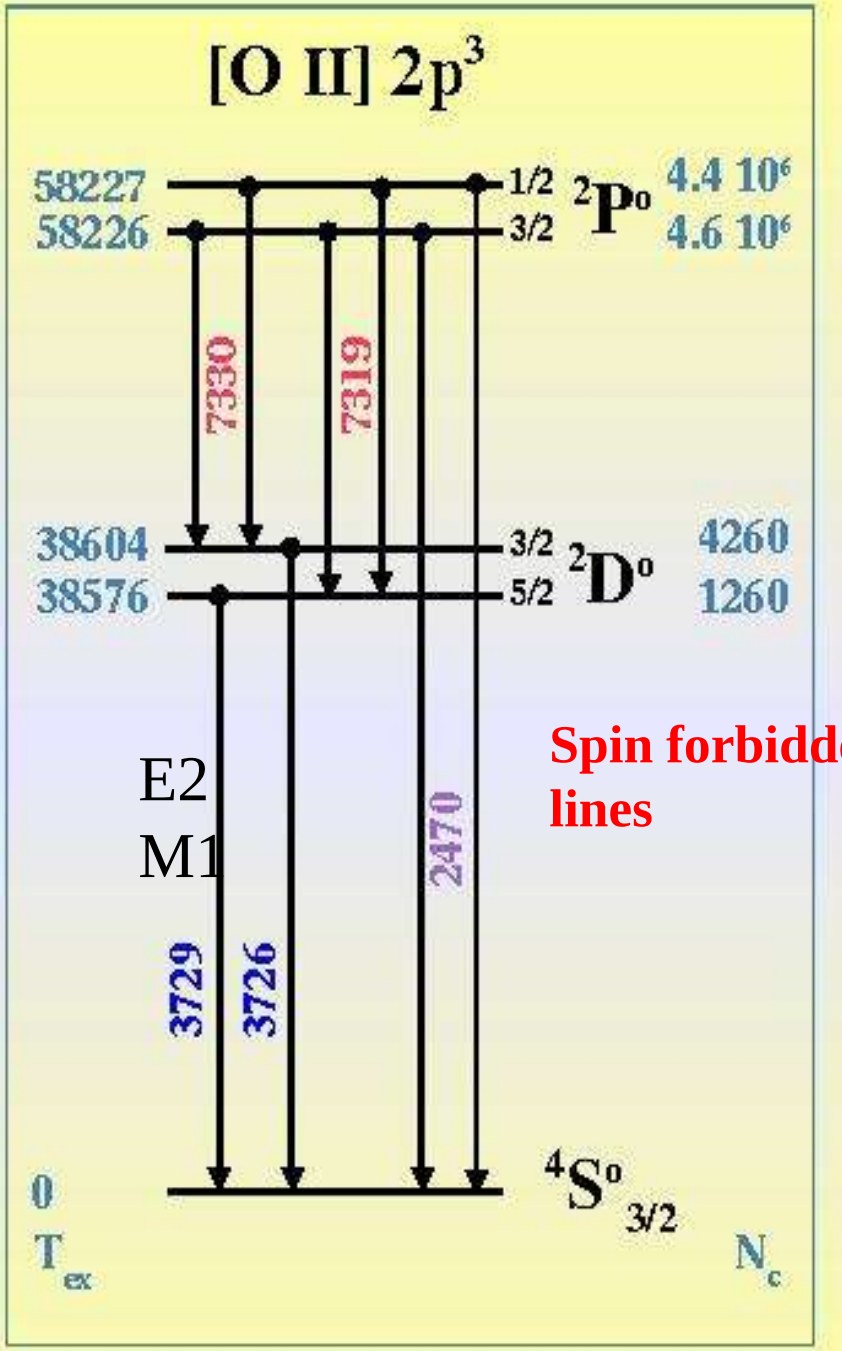
$$N_6 \xrightarrow{N_e \to 0} \frac{N_e N_0 \langle v\sigma_6 \rangle A_4}{A_6 A_4} = \frac{N_e N_0 \langle v\sigma_6 \rangle}{A_6}$$

$$N_4 = \frac{N_e^2 N_0 \langle v\sigma_{64} \rangle \left(\langle v\sigma_6 \rangle + \langle v\sigma_4 \rangle \right) + N_e N_0 \langle v\sigma_4 \rangle A_6}{N_e \left(\langle v\sigma_{46} \rangle A_6 + \langle v\sigma_{64} \rangle A_4 \right) + A_6 A_4}$$

$$N_4 \xrightarrow{N_e \to 0} \frac{N_e N_0 \langle v\sigma_4 \rangle A_6}{A_6 A_4} = \frac{N_e N_0 \langle v\sigma_4 \rangle}{A_4}$$

$$N_6 \xrightarrow{N_e \to \infty} \frac{N_e^2 N_0 \langle v\sigma_{46} \rangle \left(\langle v\sigma_6 \rangle + \langle v\sigma_4 \rangle \right)}{N_e \left(\langle v\sigma_{46} \rangle A_6 + \langle v\sigma_{64} \rangle A_4 \right)} = N_e N_0 \langle v\sigma_{46} \rangle \frac{\left(\langle v\sigma_6 \rangle + \langle v\sigma_4 \rangle \right)}{\left(\langle v\sigma_{46} \rangle A_6 + \langle v\sigma_{64} \rangle A_4 \right)}$$

$$N_4 \xrightarrow{N_e \to \infty} \frac{N_e^2 N_0 \langle v\sigma_{64} \rangle \left(\langle v\sigma_6 \rangle + \langle v\sigma_4 \rangle \right)}{N_e \left(\langle v\sigma_{46} \rangle A_6 + \langle v\sigma_{64} \rangle A_4 \right)} = N_e N_0 \langle v\sigma_{64} \rangle \frac{\left(\langle v\sigma_6 \rangle + \langle v\sigma_4 \rangle \right)}{\left(\langle v\sigma_{46} \rangle A_6 + \langle v\sigma_{64} \rangle A_4 \right)}$$



Spin forbidden lines

Density determinations

1. $N_e \to 0$

$$\frac{I(\lambda 3729)}{I(\lambda 3726)} \propto \frac{q_{^4S_{3/2},\,^2D_{5/2}}}{q_{^4S_{3/2},\,^2D_{3/2}}} \propto \frac{\omega_{^2D_{5/2}}}{\omega_{^2D_{3/2}}} = \frac{6}{4} = 1.5$$

2. $N_e \to \infty$

$$\frac{I(\lambda 3729)}{I(\lambda 3726)} \propto \frac{\omega_{^2D_{5/2}} A_{^2D_{5/2},\,^4S_{3/2}}}{\omega_{^2D_{3/2}} A_{^2D_{3/2},\,^4S_{3/2}}} = \frac{6\times 3.82\times 10^{-5}}{4\times 1.65\times 10^{-4}} = 0.35$$

Relativistic Multi-Configuration Self –Consistent Method
（准完备基方案）

$$H_{DC} = \sum_i \left[c\vec{\alpha} \cdot \vec{p}_i + (\beta - 1)c^2 - \frac{Z}{r_i} \right] + \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

$$H_{DC} \left| \Gamma PJM \right\rangle = E_\Gamma \left| \Gamma PJM \right\rangle$$

$$|\Gamma PJM\rangle = \sum_{r=1}^{n_c} c_{r\Gamma} |\gamma_r PJM\rangle$$

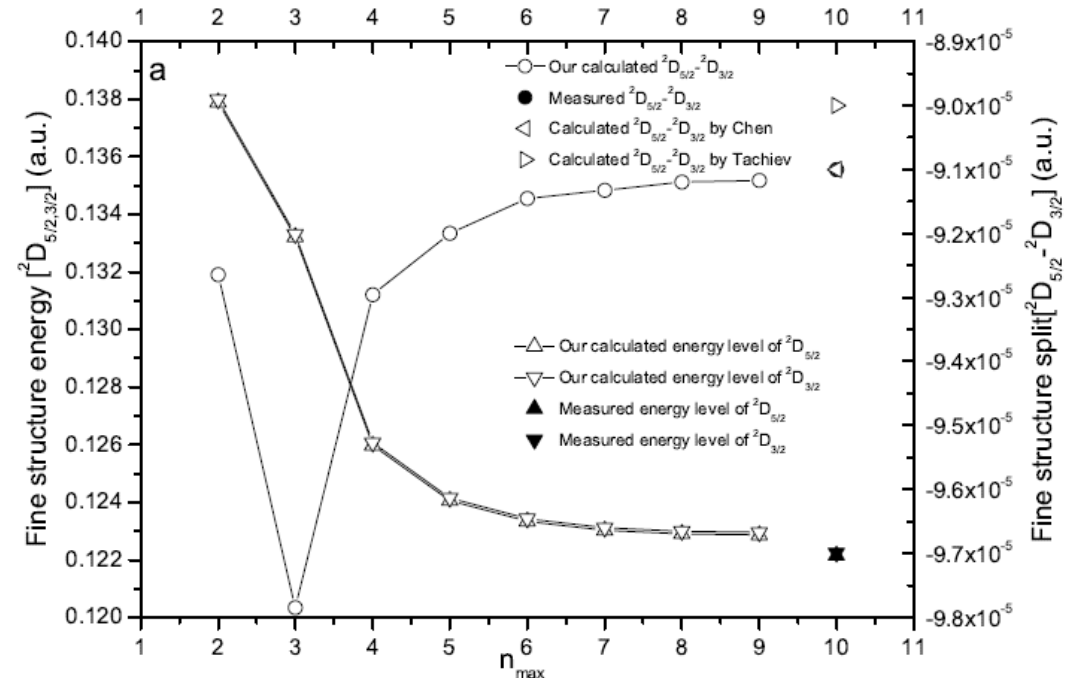
Formed by one-electron orbitals.

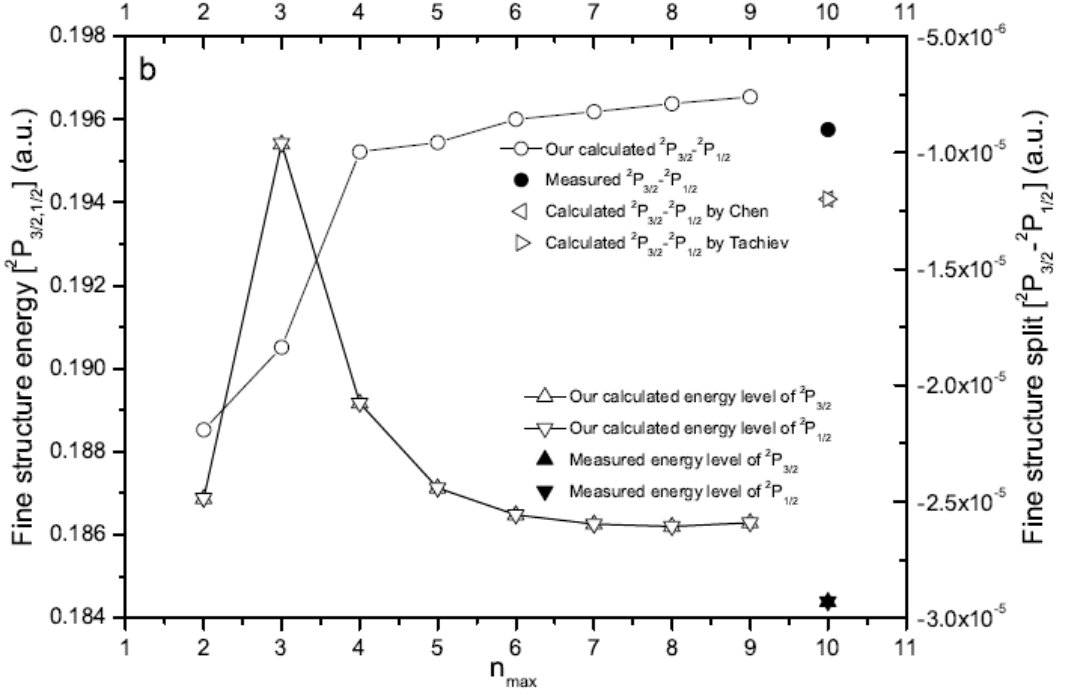
Determine the one-electron orbitals as well as C_i simultaneously.

In our calculations the CSFs of three J^π symmetries are

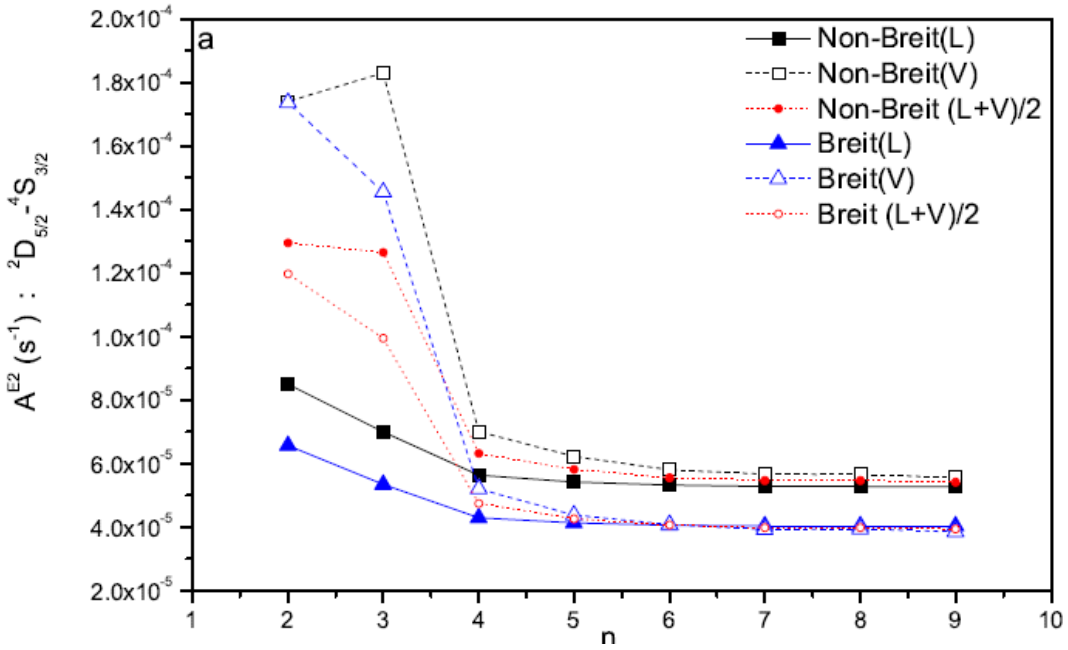
59,684($J^\pi = \left(\frac{1}{2}\right)^-$), 108,649($J^\pi = \left(\frac{3}{2}\right)^-$) , 139,620($J^\pi = \left(\frac{5}{2}\right)^-$)

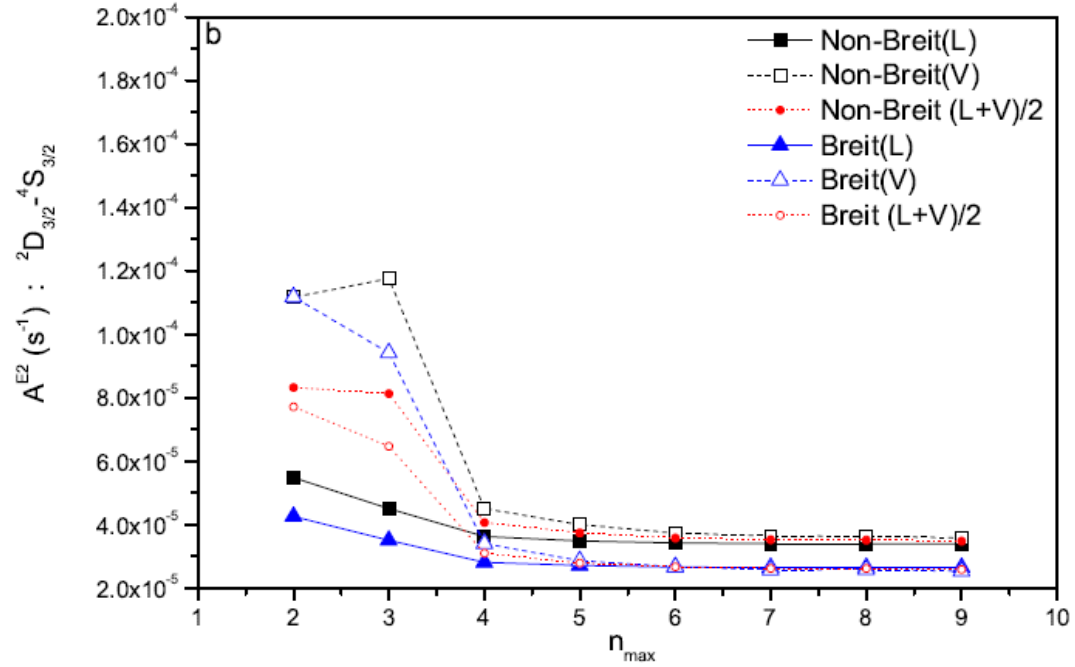
$$A_{ij} = \frac{2\pi}{2J_i + 1} \sum_{M_i, M_j} \left| \left\langle \Gamma_j P_j J_j M_j | \mathbf{T}_\lambda^{(k)} | \Gamma_i P_i J_i M_i \right\rangle \right|^2$$





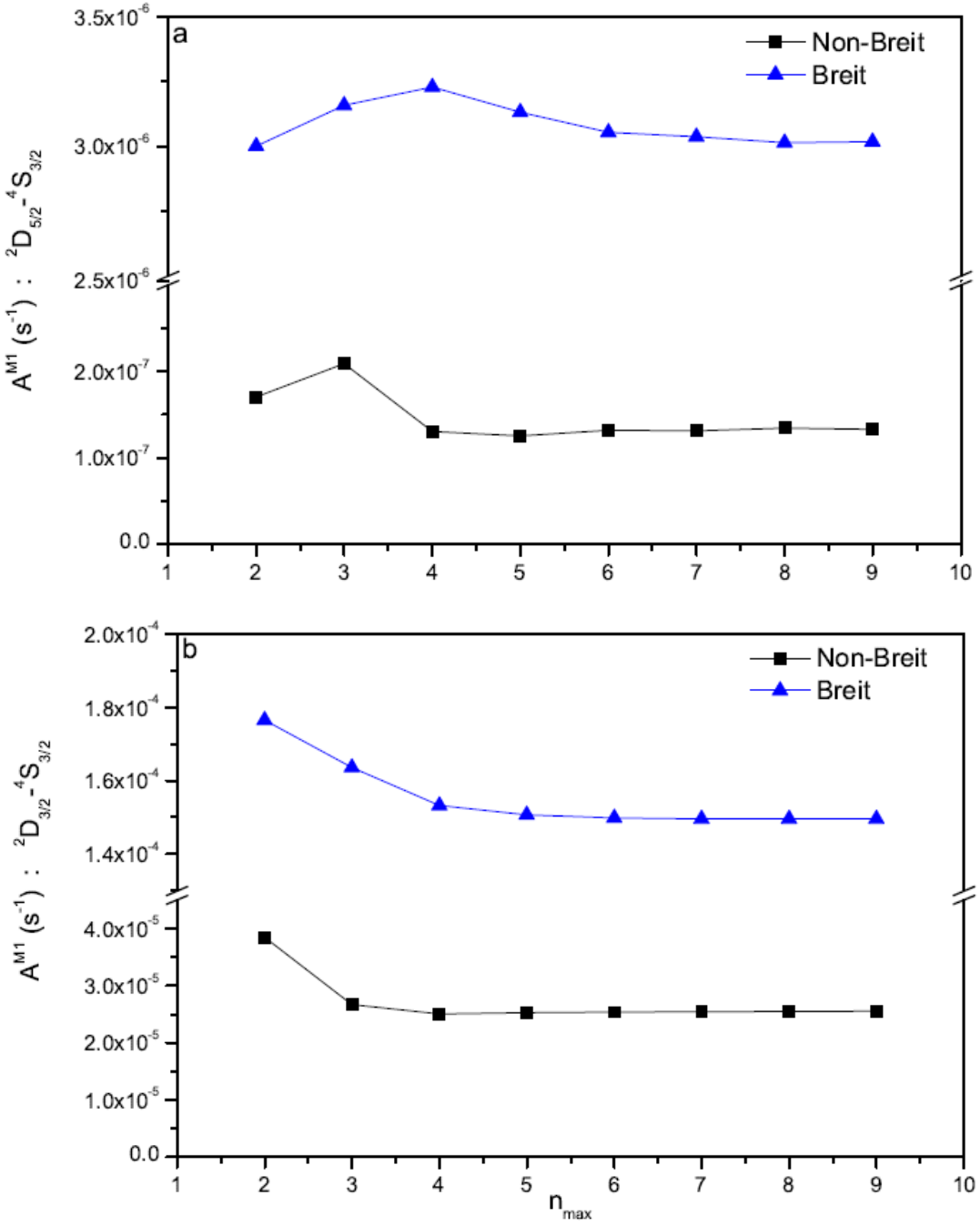
Energy level calculation of OII





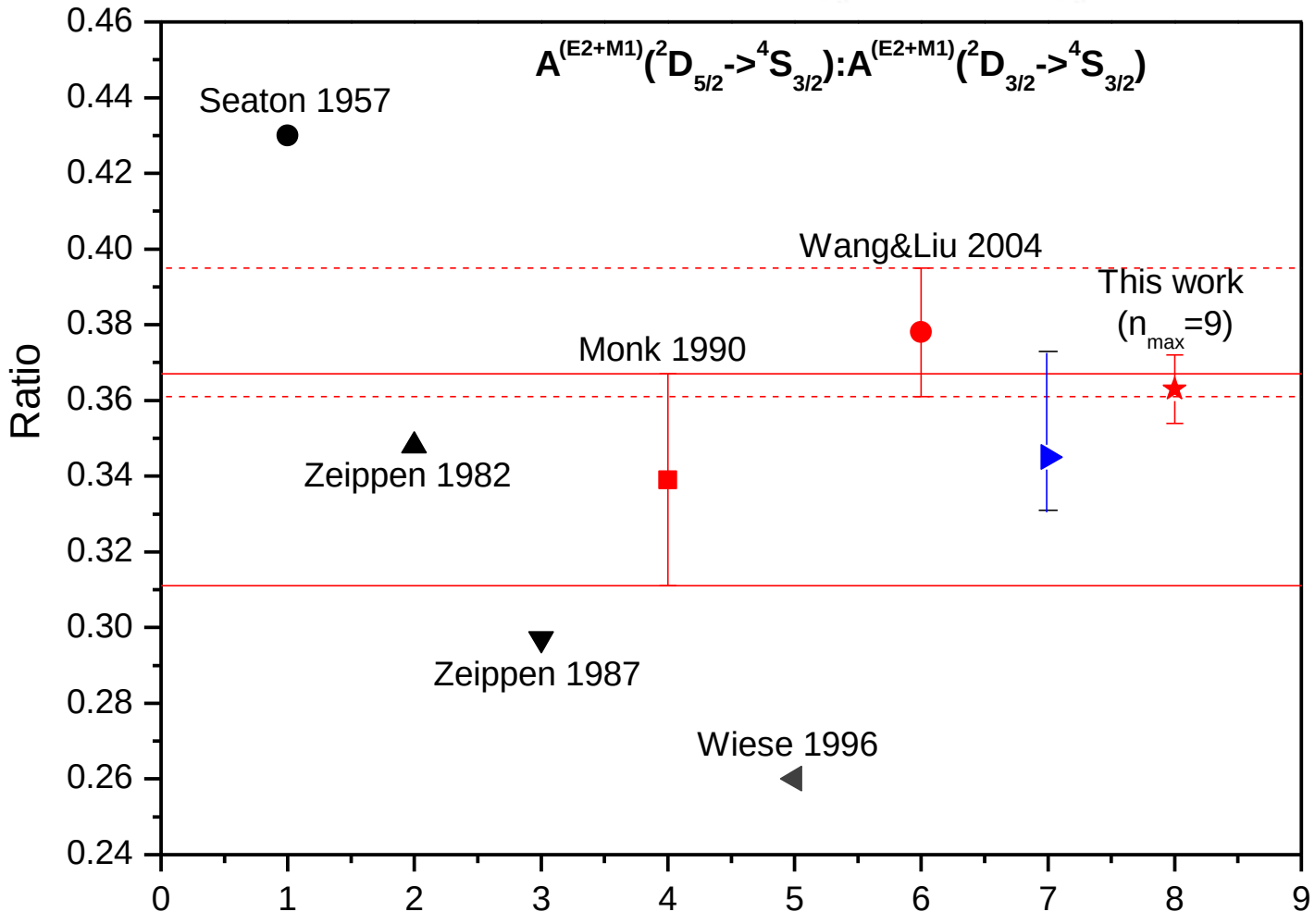
E2 transition of OII

Can estimate the errors of theoretical calculations



M1 transition of OII

$$r(\infty) = \frac{6A^{(E2+M1)}(^2D^o_{5/2} \rightarrow {}^4S^o_{3/2})}{4A^{(E2+M1)}(^2D^o_{3/2} \rightarrow {}^4S^o_{3/2})}$$

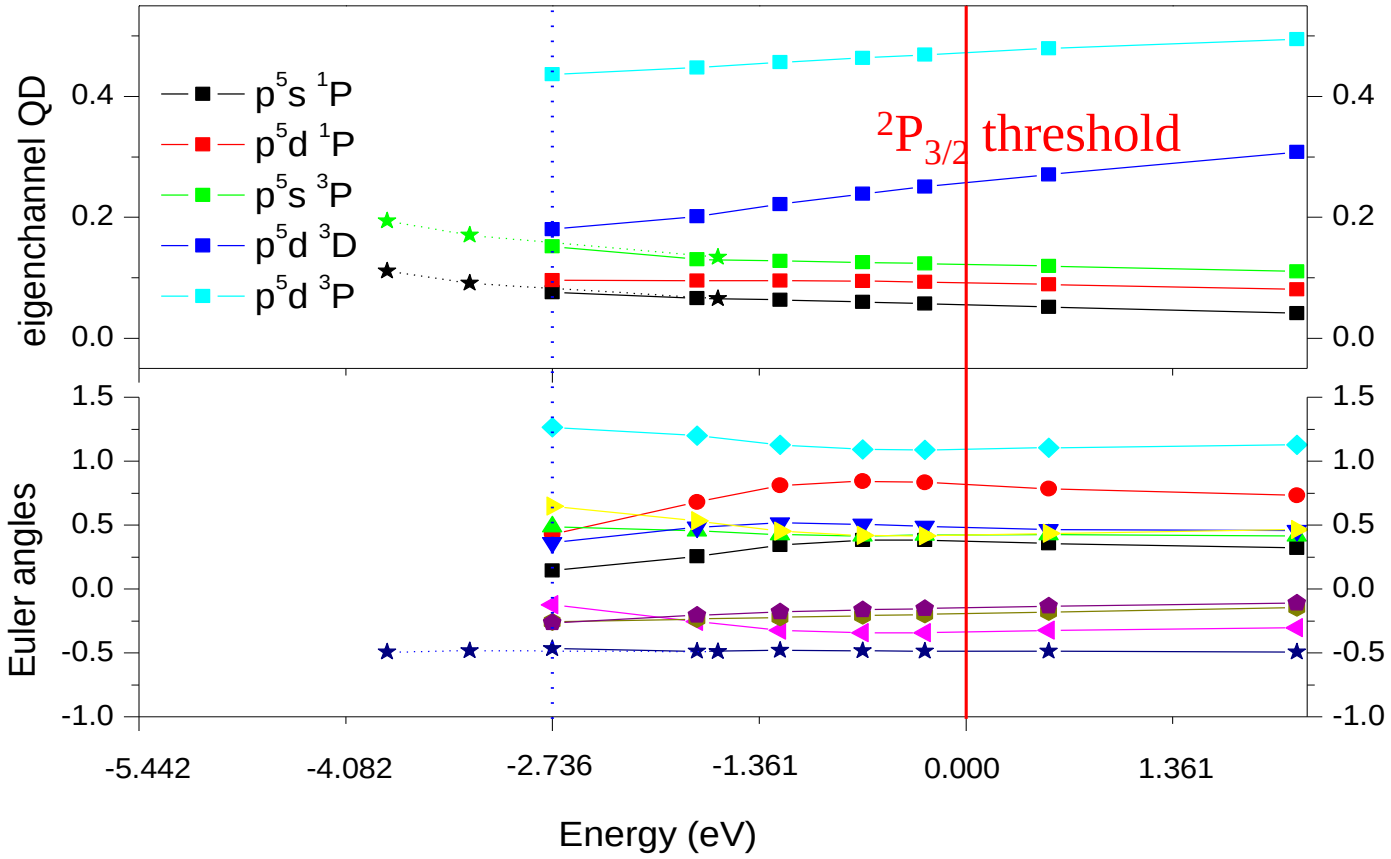


X-Y Han, X Gao, D-L Zeng, J-M Li, Phys. Rev. A 85 (2012), 062506

Transition	Type	This work($n_{max}=9$)	Chen 2007 [a]	Zeippen 1982 [b]	Zeippen 1987 [c]	Fischer& Tachiev 2004 [d]
$^2D^o_{5/2} \rightarrow {}^4S^o_{3/2}$	E2	$3.94^{+0.09}_{-0.09}(-5)$	$3.91^{+0.08}_{-0.11}(-5)$	3.64(-5)	3.39(-5)	3.382(-5)
	M1	$3.02^{+0.08}_{-0.08}(-6)$	$3.00^{+0.06}_{-0.06}(-6)$	1.83(-6)	1.98(-6)	7.416(-6)
	E2+M1	$4.25^{+0.10}_{-0.10}(-5)$	$4.21^{+0.09}_{-0.11}(-5)$	3.82(-5)	3.59(-5)	4.124(-5)
$^2D^o_{3/2} \rightarrow {}^4S^o_{3/2}$	E2	$2.59^{+0.06}_{-0.06}(-5)$	$3.48^{+0.20}_{-0.99}(-5)$	2.36(-5)	2.20(-5)	2.209(-5)
	M1	$1.50^{+0.04}_{-0.04}(-4)$	$1.48^{+0.01}_{-0.00}(-4)$	1.41(-4)	1.59(-4)	1.414(-4)
	E2+M1	$1.75^{+0.05}_{-0.05}(-4)$	$1.83^{+0.03}_{-0.10}(-4)$	1.65(-4)	1.81(-4)	1.635(-4)
$^2P^o_{3/2} \rightarrow {}^4S^o_{3/2}$	E2	$1.27^{+0.10}_{-0.10}(-6)$				1.233(-8)
	M1	$5.87^{+0.44}_{-0.44}(-2)$				5.646(-2)
	E2+M1	$5.87^{+0.44}_{-0.44}(-2)$				5.646(-2)
$^2P^o_{1/2} \rightarrow {}^4S^o_{3/2}$	E2	$5.27^{+4.16}_{-4.16}(-8)$				1.510(-6)
	M1	$2.35^{+1.85}_{-1.85}(-2)$				2.265(-2)
	E2+M1	$2.35^{+1.85}_{-1.85}(-2)$				2.265(-2)

spin flip **E^2 Δ L=2** **M^1 Δ L=1**

Multi-Channel Example: $e+Kr^+$



$e + Kr^+(^2P_{3/2,1/2})$; $J^\pi = 1^-$; $S_{ij}(5\times5)$; $5\,\mu_\alpha$, $U_{i\alpha}(5\times5) \Leftrightarrow 10\,\theta_{i\alpha}$

$J^\pi = 1^-$; 3 channels $Kr^+(^2P_{3/2}) + e(s_{1/2}, d_{5/2}, d_{3/2})$

2 channels $Kr^+(^2P_{1/2}) + e(s_{1/2}, d_{3/2})$

$$S_{ij} = \sum_{\alpha}^{N} U_{i\alpha} \exp\left(i\, 2\pi\mu_{\alpha}\right) U_{j\alpha} \qquad N \times N \text{ matrix}$$

$$\Psi = \sum_{\alpha} A_{\alpha} \Psi_{\alpha}$$

Bound states **electron scattering processes**

$$F(\{\nu_i\};\{U_{i\alpha};\mu_{\alpha}\}) = \det\left[U_{i\alpha} \sin \pi(\nu_i + \mu_{\alpha})\right] = 0 \qquad (1)$$

$$E = I_i - \frac{(q+1)^2}{2\nu_i^2}, \quad \text{for all } i \qquad (2)$$

$$e^{i\sigma_i} \cdot S_{ij} \cdot e^{i\sigma_j}$$

Multichannel Quantum Defect Theory **σ Coulomb phase shift**

Let us look a simple case; namely, N=1, q=0

$$\sin \pi(\nu + \mu) = 0$$

$$\nu + \mu = n$$

$$\nu_n = n - \mu$$

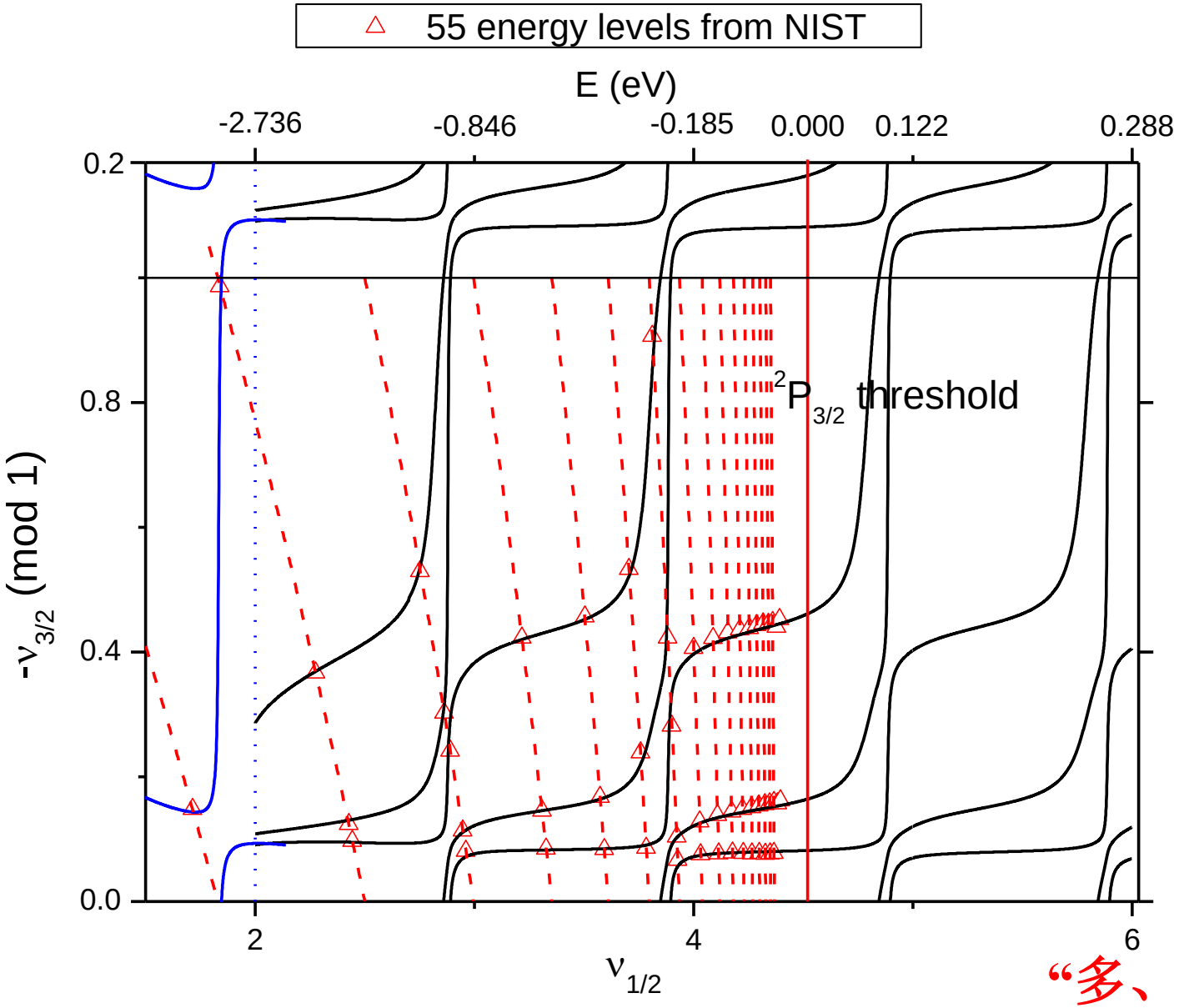
$$\exp[i\, 2(\pi\mu + \sigma)]$$
$$= \exp[i\, 2(\delta + \sigma)]$$

Rydberg formula

$$E_n = I - \frac{(q+1)^2}{2\nu_n^2} = I - \frac{1}{2(n-\mu_n)^2}$$

$$\lim_{n\to\infty} \pi\mu_n = \delta(0)$$

Graphical illustration of the solution of Eq.(1) and Eq.(2)



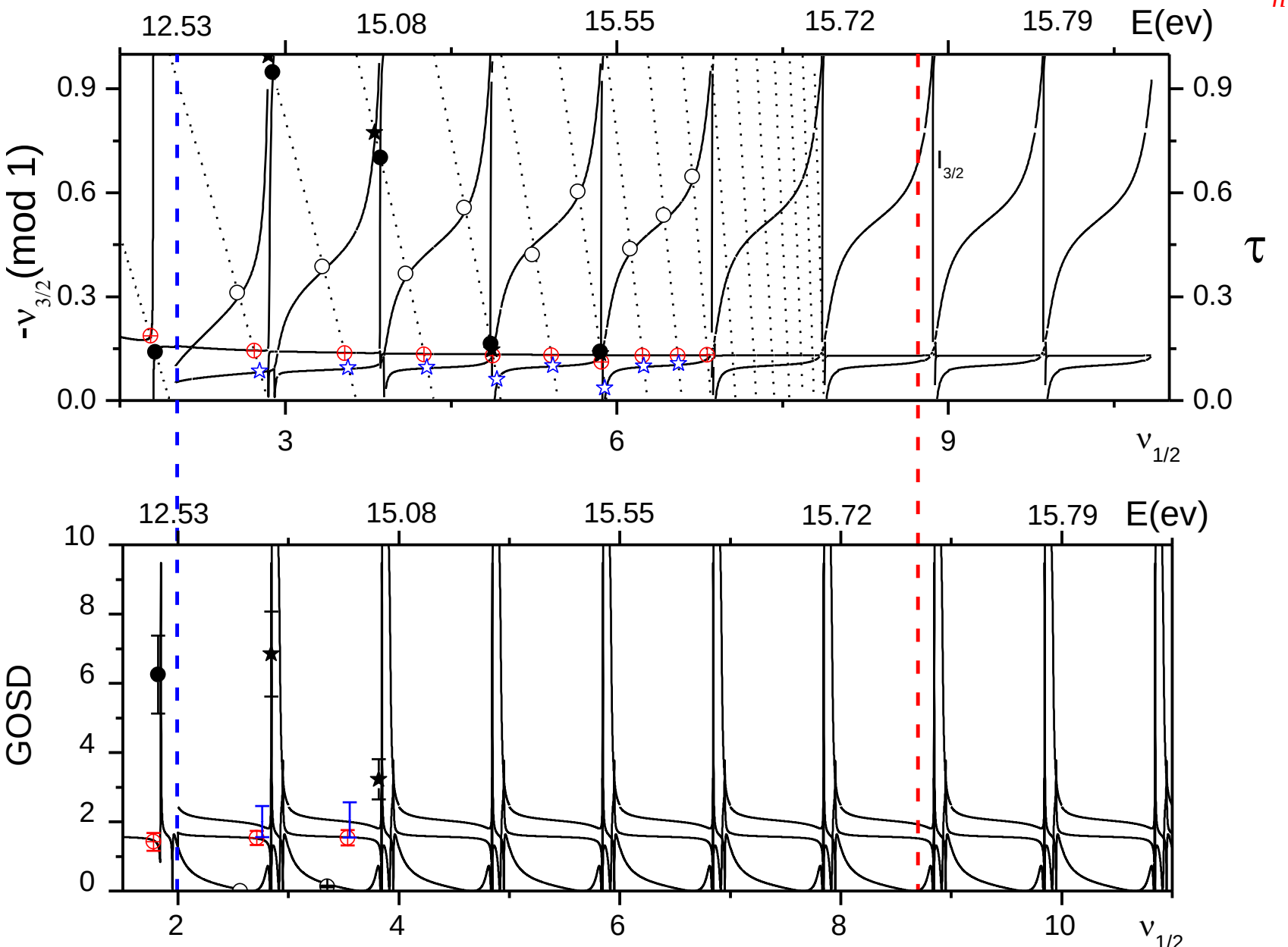
All bound energy levels without missing any one.

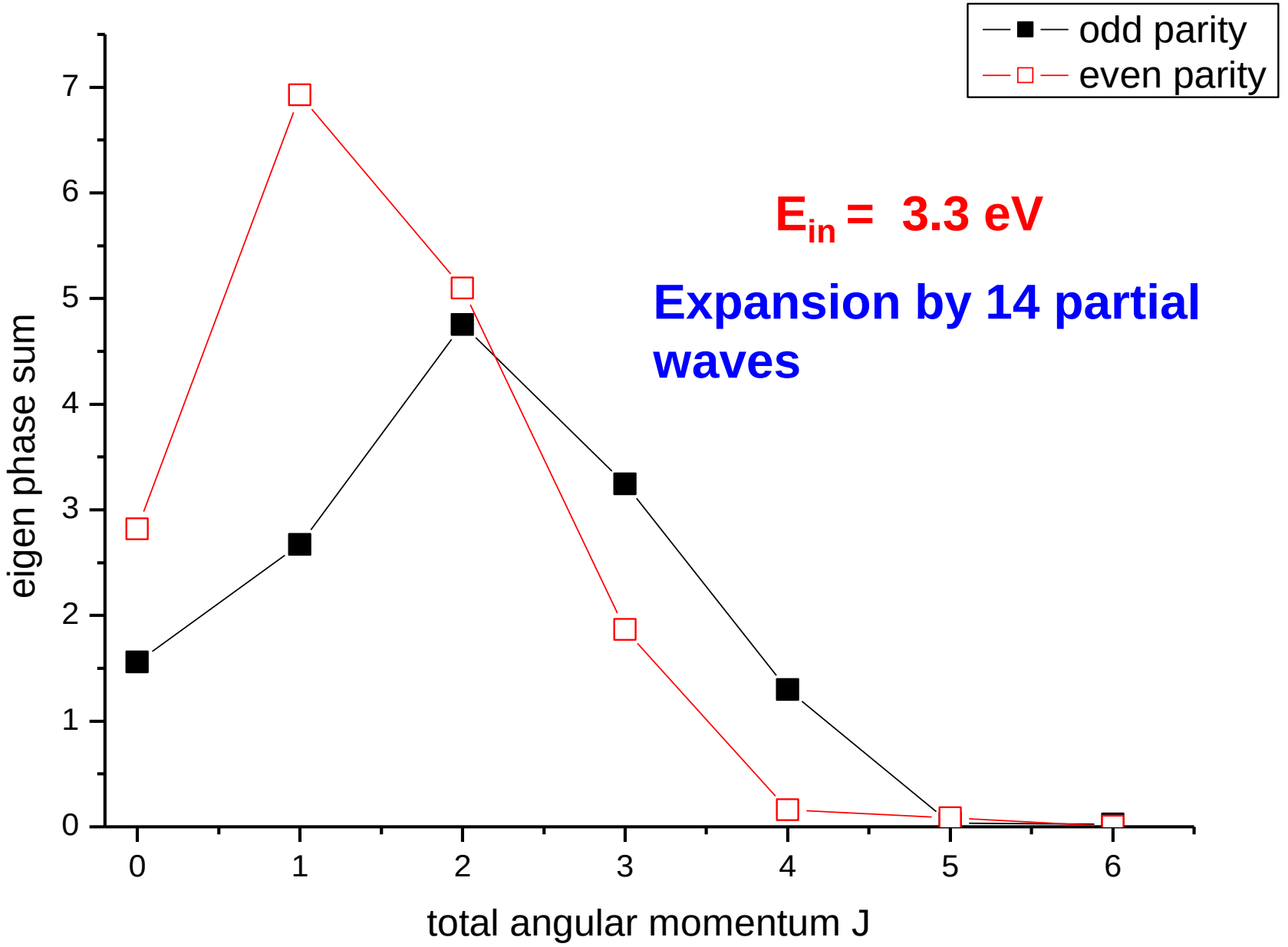
The precision spectroscopic spectrums can then be served as stringent tests of the accuracy of the short-range scattering matrices

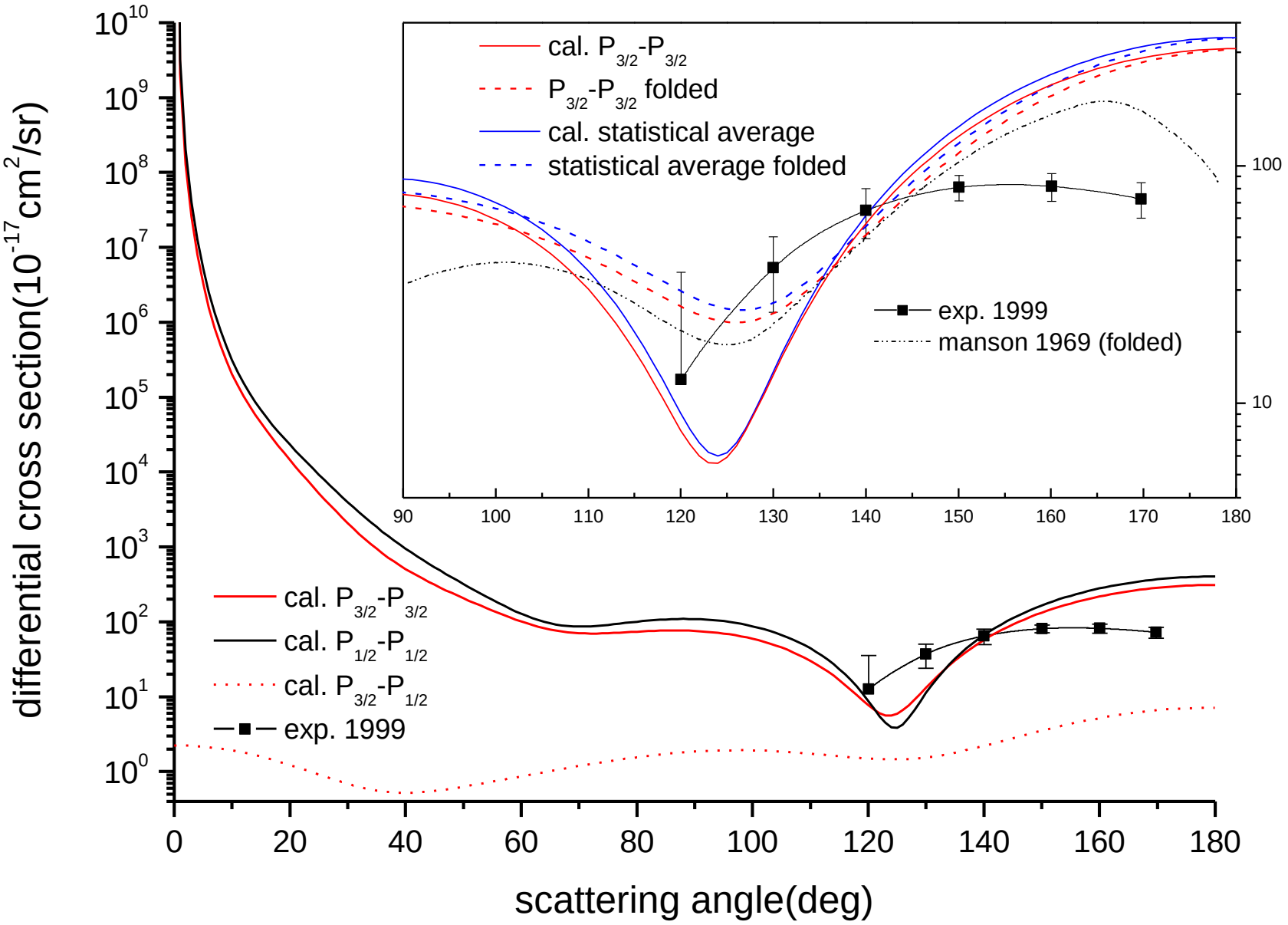
“多、快、好、省”

Optical Processes（Optical Oscillator Strength Densities OSD）

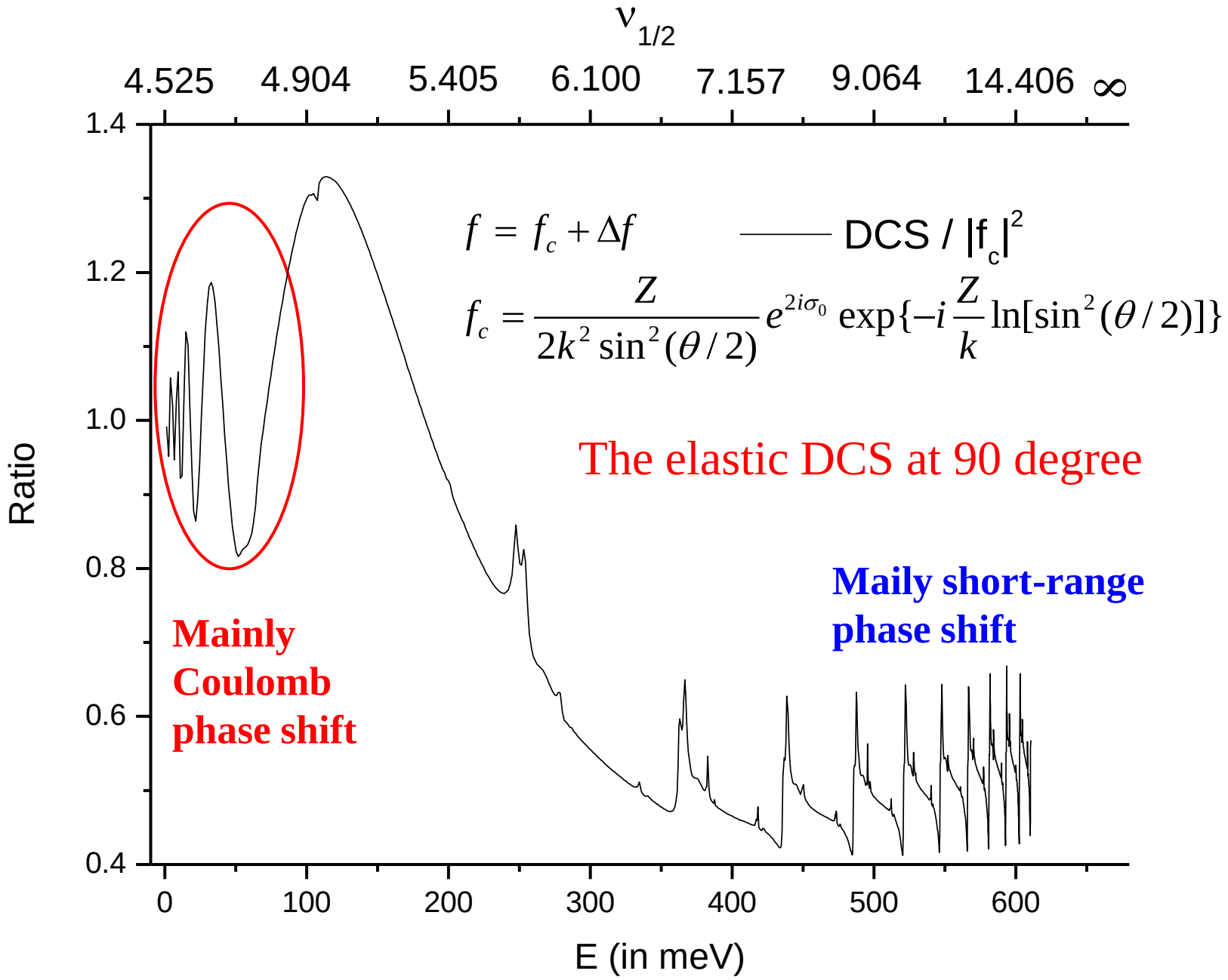
$$h\nu + A \rightarrow A_n^*$$



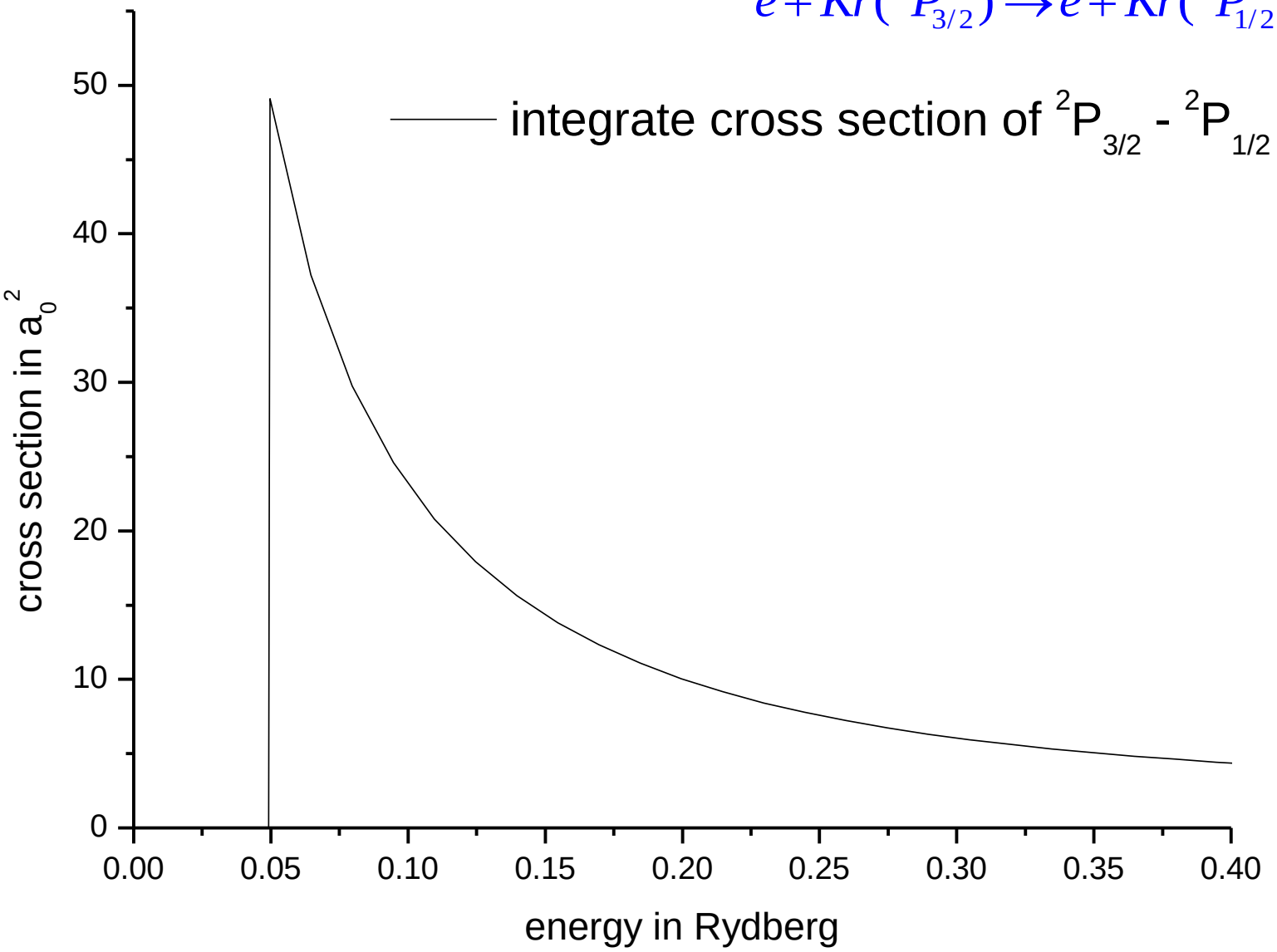

odd parity
even parity
E_{in} = 3.3 eV
Expansion by 14 partial waves
eigen phase sum
total angular momentum J
0
1
2
3
4
5
6
7


E_{in} = 3.3 eV
differential cross section(10^{-17}cm^2/sr)
scattering angle(deg)
cal. $P_{3/2}$-$P_{3/2}$
cal. $P_{1/2}$-$P_{1/2}$
cal. $P_{3/2}$-$P_{1/2}$
exp. 1999
$P_{3/2}$-$P_{3/2}$ folded
cal. statistical average
statistical average folded
manson 1969 (folded)

Provide some physical systems to test the energy resolution of the electron beam in merged-beam facilities



$$e + Kr(^2P_{3/2}) \rightarrow e + Kr(^2P_{1/2})$$



radiative cooling

The high-energy electron impact excitation differential cross sections can be written as Born approximation,

$$\frac{d\sigma_n}{d\Omega} = \frac{k'}{k}\left| f_n^B(\hat{k},\hat{k}')\right|^2 = \frac{2}{\Delta E_n}\frac{k'}{k}\frac{F_n(\Delta E_n, K)}{K^2}$$

GOS

$$F_n(\Delta E_n, K) = \frac{K^2\cdot\Delta E_n}{2}\left| f_n^B(\hat{k},\hat{k}')\right|^2$$

$$e_i + \mathrm{A} \rightarrow e_f + \mathrm{A}_n^*$$

$$= \frac{2\Delta E_n}{K^2\cdot N_n^2}\left|\left\langle\Psi(E_n)\right|\sum_{j=1}^{N} e^{i\vec{K}\cdot\vec{r}_j}\left|\Psi_0\right\rangle\right|^2$$

$$= \frac{2\Delta E_n}{K^2\cdot N_n^2}\left|\sum_{\alpha} G_\alpha\cdot A_{\alpha,n}\right|^2$$

$$\boldsymbol{G_\alpha} = <\psi_\alpha\left|\sum_{\boldsymbol{j}=1}^{\boldsymbol{N}}\boldsymbol{e}^{\boldsymbol{i\vec{K}\cdot\vec{r}_j}}\right|\Psi_{\boldsymbol{o}}>$$

GOSD

$$\frac{dF_{n,\rho}(\Delta E_n, K)}{dE} = \frac{2\left(E-E_0\right)\left|\sum_\alpha G_\alpha A_{\alpha,n,\rho}\right|^2}{N_{3/2,n,\rho}^2}$$

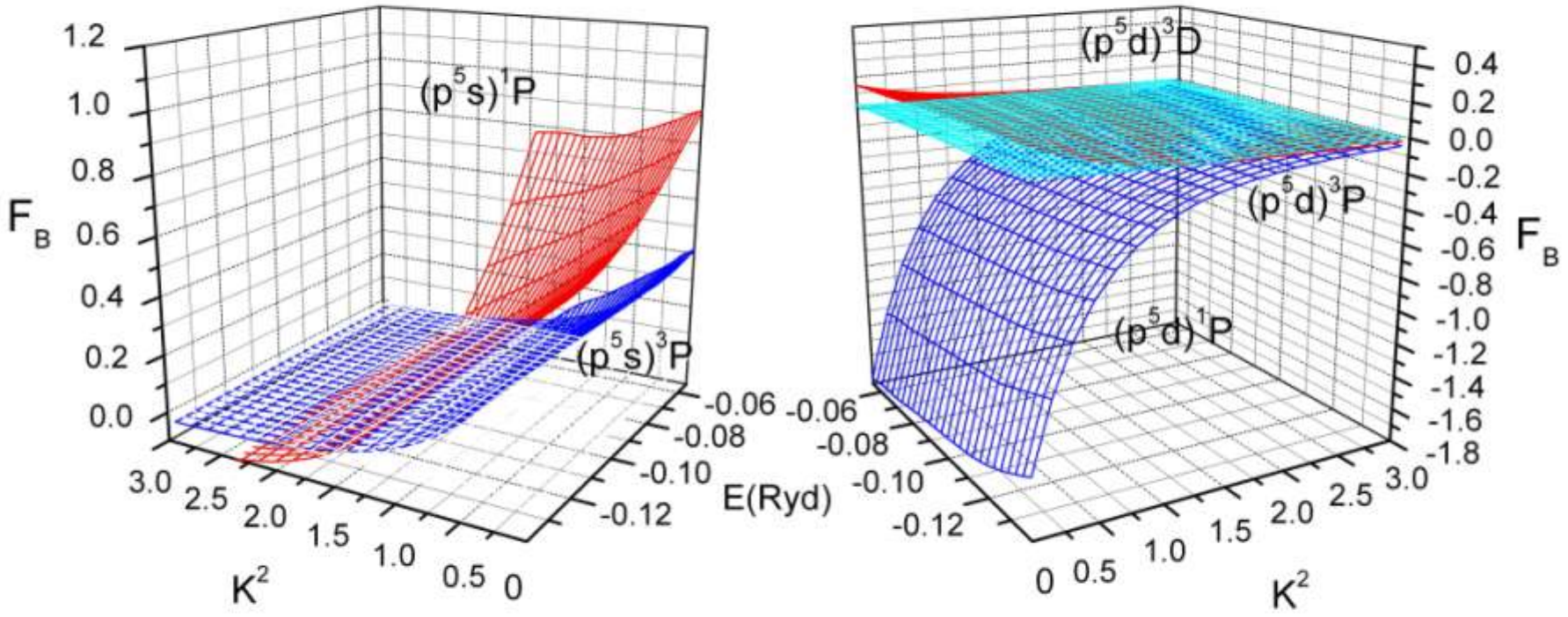
The calculation of GOS by eigenchannel wavefunctions

OS : $Ar(3p^6) + h\nu -> Ar^*(3p^5 n/\varepsilon\ s,d)$ $\sim \langle \Psi_\alpha | r | \Psi_0 \rangle$

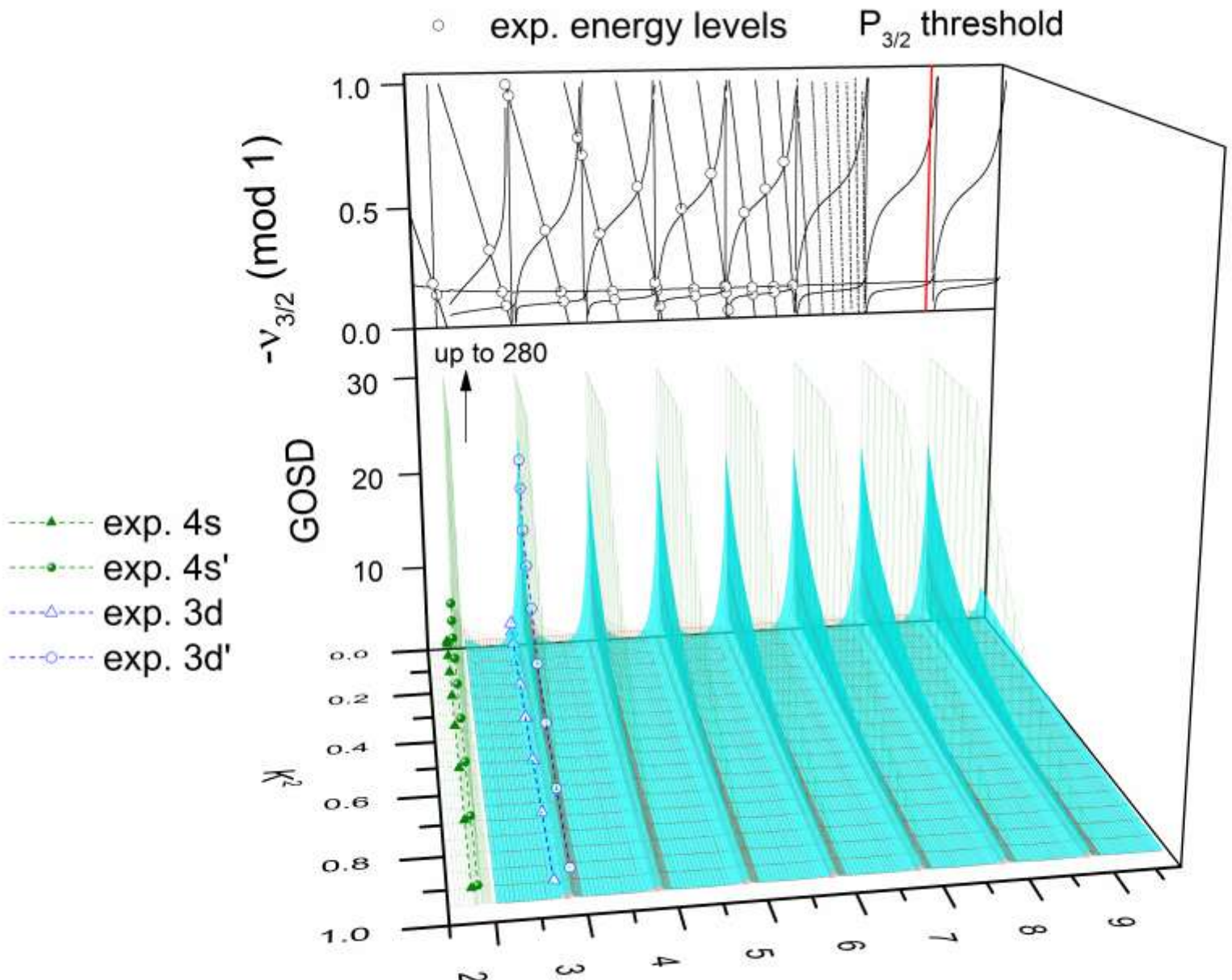
GOS : $e + Ar(3p^6) -> e + Ar^*(3p^5 n/\varepsilon l)$ $\sim \langle \Psi_\alpha | e^{iKr} | \Psi_0 \rangle$ Born approximation

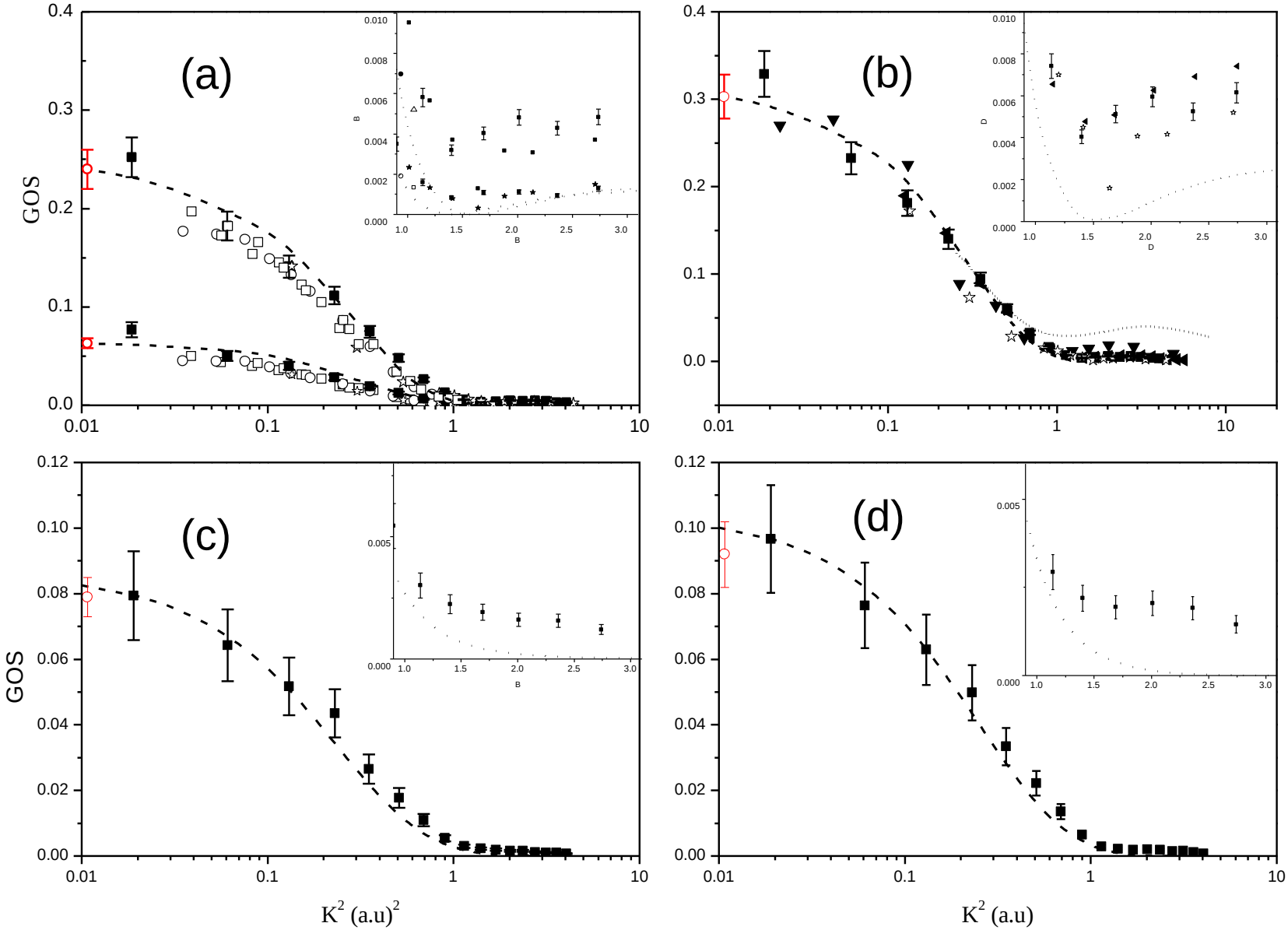
All n/ε(infinite) are needed !

Ψ_α: $J^\pi = 1^-$; 5 eigenchannels: $(p^5 s)\ ^1P$ $(p^5 s)\ ^3P$ $(p^5 d)\ ^3D$ $(p^5 d)\ ^3P$ $(p^5 d)\ ^1P$



The GOSD for physical states—Born approximation of high energy electron-ion scatterings





The GOS's to the excitations to (a) 4s[3/2] and 4s[1/2], (b) sum of 4s, (c) 3d[3/2] and (d) 3d[1/2].

○ Li *et al.* at 400eV; ☆ Li *et al.* at 500eV; ■ Bielschowsky *et al.* at 1000eV; ○ Ji *et al.* at 1500eV; ☆ Fan and Leung at 2500eV; Zhu *et al.* at 2500eV; □ Wong *et al.* at 25keV;- - - · present results.

L.F. Zhu, et. al. Phys. Rev. A, 73, 042703 (2006).

Summary

- **We develop the R-Eigen/R-R-Eigen code to directly calculate short-range scattering matrices with good analytical properties in the whole energy regions, from which we can obtain all energy levels and the related scattering cross sections with accuracies comparable with spectroscopic precision. Such code can provide necessary abundant atomic data with enough accuracies for relevant research fields, such as inertial confinement fusion researches and astrophysics studies.**
- 能找到相互切入点吗？

感谢我们研究团队的年轻同志

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谢谢！