

ab initio Relativistic Many-Body
studies on electronic structure of
 Ti^{3+}

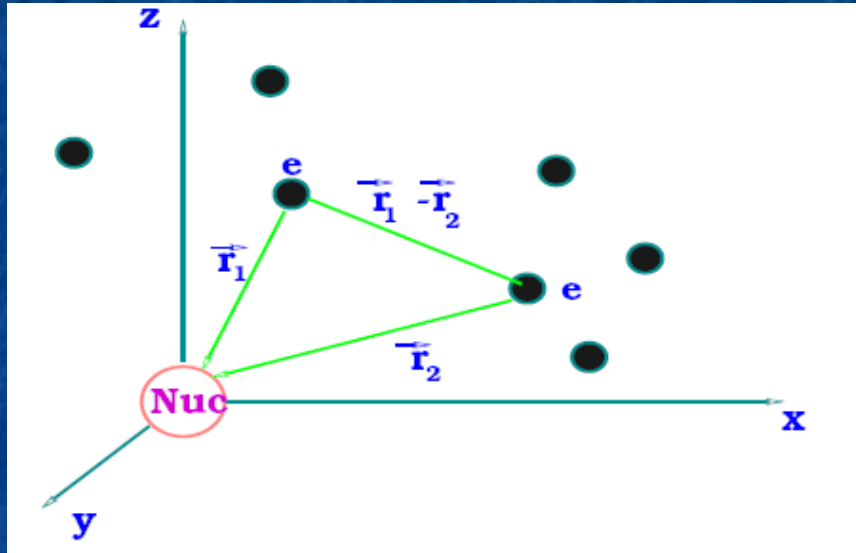
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Plan of Presentation

- Introduction
- Motivation
- Theory
- Results
- Conclusion

Atomic Many-Electron Processes



Hamiltonian = K.E. + Nuclear Attraction + Coulomb Repulsion

Schrödinger Equation \rightarrow Wavefunction

Wavefunction \rightarrow Any atomic property
importance

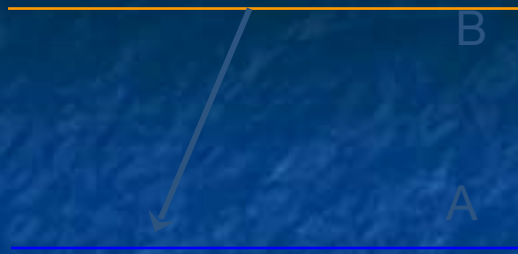
Experimental difficulties $\rightarrow\rightarrow$ Dependence on theoretical study

Need For accurate wave length ,energy value and f- value

- Reliable line identification
- Finding unknown energy levels
- Forbidden transitions are important in nebular and Circumstellar and SN studies.
- Calculation in the search of electron's EDM



Astrophysics: Spectrum Synthesis : Curve – of – Growth analysis

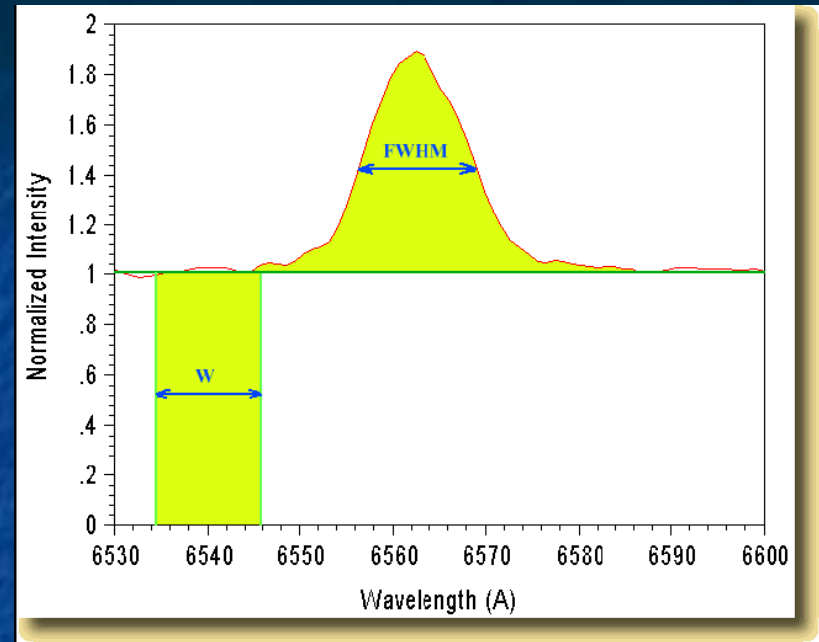


Intensity of spectrum

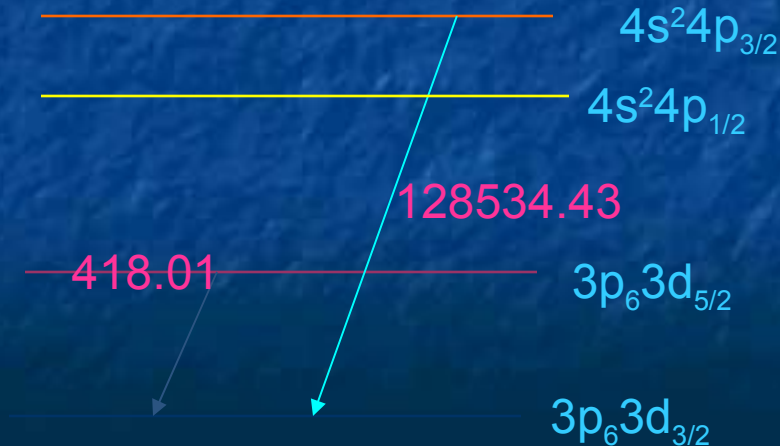
\propto no. of absorbing/emitting atom

\propto no. atoms available (N) $\times f_{AB}$

$$\log X = \log gf + \log \Gamma + \log \frac{N_{Ti}}{N_H}$$



Ti IV



Wolf-Rayet Star

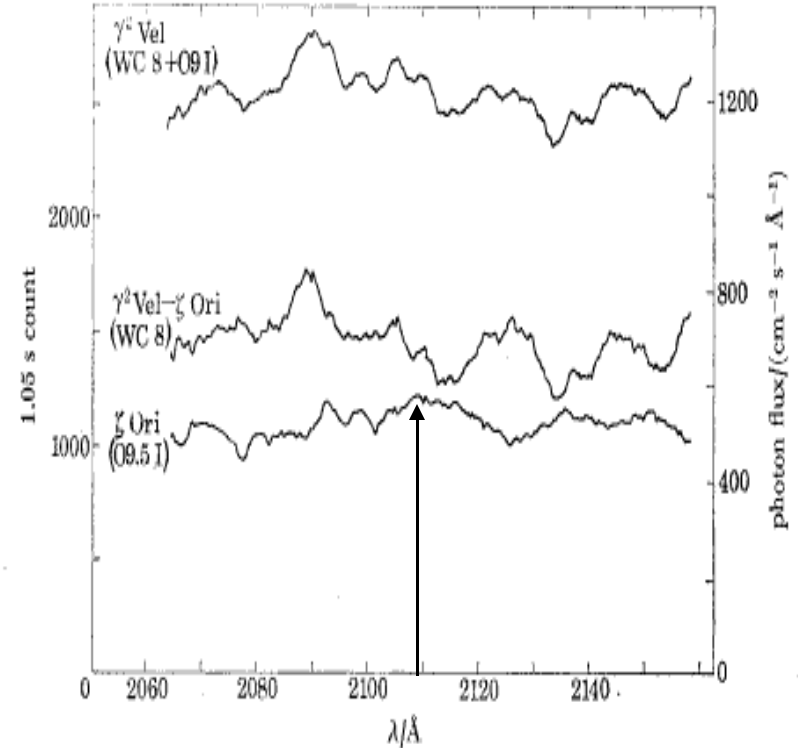


FIGURE 1. S59 2100 Å channel. Spectra of γ^2 Vel (WC8+O9 I), May 1972, an O9.5 I star (ζ Ori) and resulting WC8 star. The ordinates do not refer to the actual observation of ζ Ori but to the γ^2 Vel system.

Space Research Lab of the
 astronomical Institute
 ,Netherlands
 (Phil.Trans.R.Soc. land
 A,279,(1975)

Radiative Transition Selection Rule

Transition	Parity	ΔJ	ΔS
E1(allowed)	Yes	0, ± 1	0
M1(Forbidden)	No	0, ± 1	0
E2(Forbidden)	No	0, ± 1 , ± 2	0

Expressions of Transition amplitudes

Transition probability

$$\begin{aligned}
 A_{\beta \rightarrow \alpha} &= [j_\beta] \sum_{M_\beta} \sum_{M_\alpha} 2\pi |M_{\alpha\beta}|^2 \\
 &= 2\alpha\omega \frac{[j_\alpha]}{[L]} \left(\begin{array}{ccc} j_\beta & L & j_\alpha \\ 1/2 & 0 & -1/2 \end{array} \right)^2 |\overline{M_{\alpha\beta}}|^2
 \end{aligned}$$

Using 3-j symbol

Oscillator Strength

$$f_{\beta \rightarrow \alpha} = \frac{[j_\beta] A_{\beta \rightarrow \alpha}}{[j_\alpha] 2\alpha \omega^2}$$

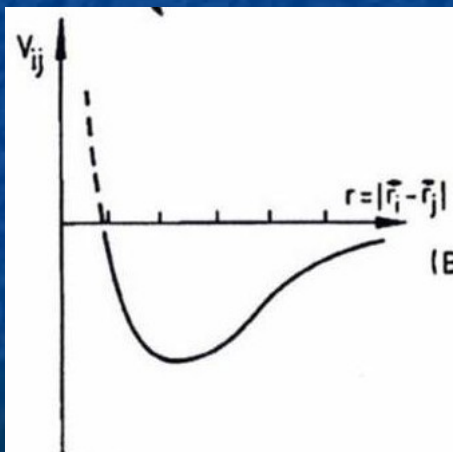
Hamiltonian of Electronic system

$$H^{\text{Rel.}} = \sum_i \left[c\vec{\alpha} \cdot \vec{p}_i + (\beta - 1)c^2 \right] - \sum_{i,A} Z_A r_{iA}^{-1} + \sum_{i>j} r_{ij}^{-1}$$

One-Body Part
(K.E. Of Electrons,
Nucl. Attraction)

Two-Body Part

(Repulsions
among electrons)



Dirac-Fock Approximation
(Relativistic form of HF)

Correlation

Perturbative

Non-Perturbative

- Effective Valence Shell Model (HV)
- Multi-Configuration Perturbation (MCPT)

- Multi-configuration DF(MCDF)
- Coupled Cluster Method (CC)
- Density Functional Theory (DFT)

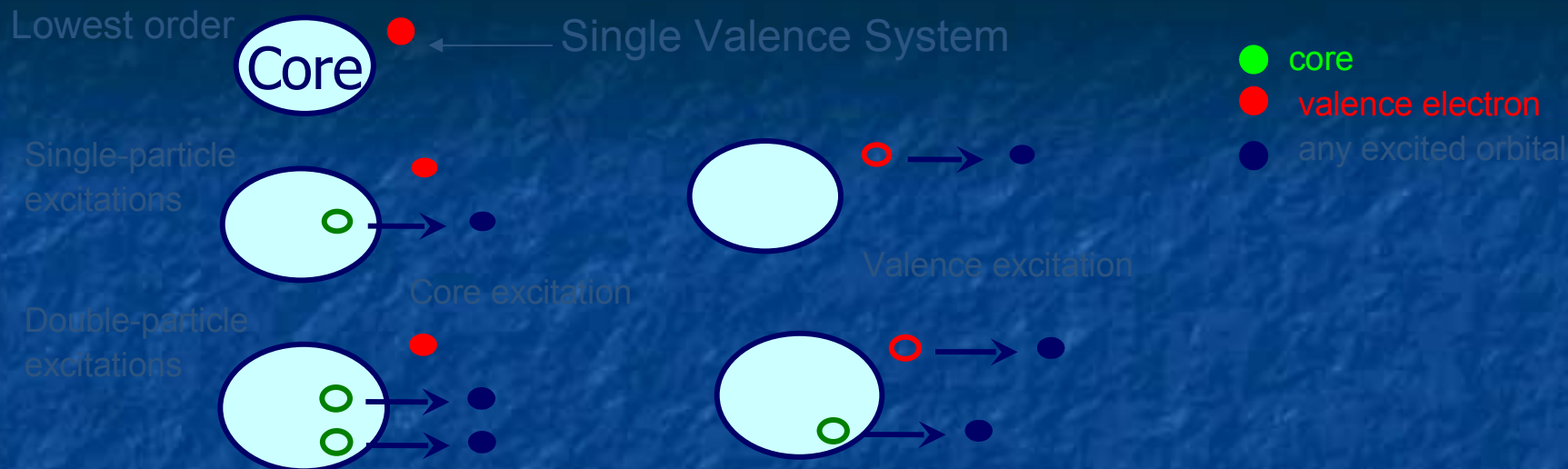
- Have to Go beyond Hartree-Fock



- DF Potential



Development & calculation using Coupled Cluster Method



$$S_2 |\Phi_0\rangle = \sum_{abpq} s_{ab}^{pq} a_p^+ a_q^+ a_b a_a |\Phi_0\rangle$$

$$S_1 |\Phi_0\rangle = \sum_{ap} s_a^p a_p^+ a_a |\Phi_0\rangle$$

$$|\Psi\rangle = e^{S_1 + S_2} |\Phi_0\rangle$$

ab initio, highly correlated MB method

Phys. Today, April 1997, July 2001, June 2003

Motivation : Highly accurate calculations for BEC, Parity Non-Conservation in atom, EDM of electron

Developed massively parallelized relativistic CC code

Need High Performance Computing

$$|\Psi\rangle = e^S |\Phi_0\rangle,$$

Where, $S = S_1 + S_2 + \dots$

Schödinger Equation :

$$H|\Psi\rangle = E|\Psi\rangle \Rightarrow H e^S |\Phi_0\rangle = E e^S |\Phi_0\rangle$$

Define Normal Order Hamiltonian :

$$\tilde{H} \equiv H - \langle \Phi_0 | H | \Phi_0 \rangle = H - E_{DF}$$

$$\tilde{H} e^S |\Phi_0\rangle = (E - E_{DF}) e^S |\Phi_0\rangle \equiv E_{corr} e^S |\Phi_0\rangle$$

$$\langle \Phi_0 | e^{-S} \tilde{H} e^S | \Phi_0 \rangle = E_{corr}$$

$$\langle \Phi_0^* | e^{-S} \tilde{H} e^S | \Phi_0 \rangle = 0$$

CCSD approximation: $S = S_1 + S_2 \rightarrow$

$$A + B(S) \cdot S = 0$$

where $A = \langle \Phi_0^* | \tilde{H} | \Phi_0 \rangle$.

Since, $B(S)$ depends on Cluster amplitudes,

\Rightarrow Solve Self-consistently.

$$|\psi_v\rangle = e^T e^s |\phi_v\rangle = e^T \{1 + S\} |\phi_v\rangle$$

New Reference state $|\varphi_v\rangle = a^+ |\varphi_{DF}\rangle$

$$D_{fi} = \frac{\langle \psi_f | D | \psi_i \rangle}{\langle \psi_f | \psi_i \rangle} = \frac{\langle \varphi_f | \{1 + S_f\} e^{T^+} D e^T \{1 + S_i\} |\varphi_i\rangle}{\langle \varphi_f | \{1 + S_f\} e^{T^+} e^T \{1 + S_i\} |\varphi_i\rangle}$$

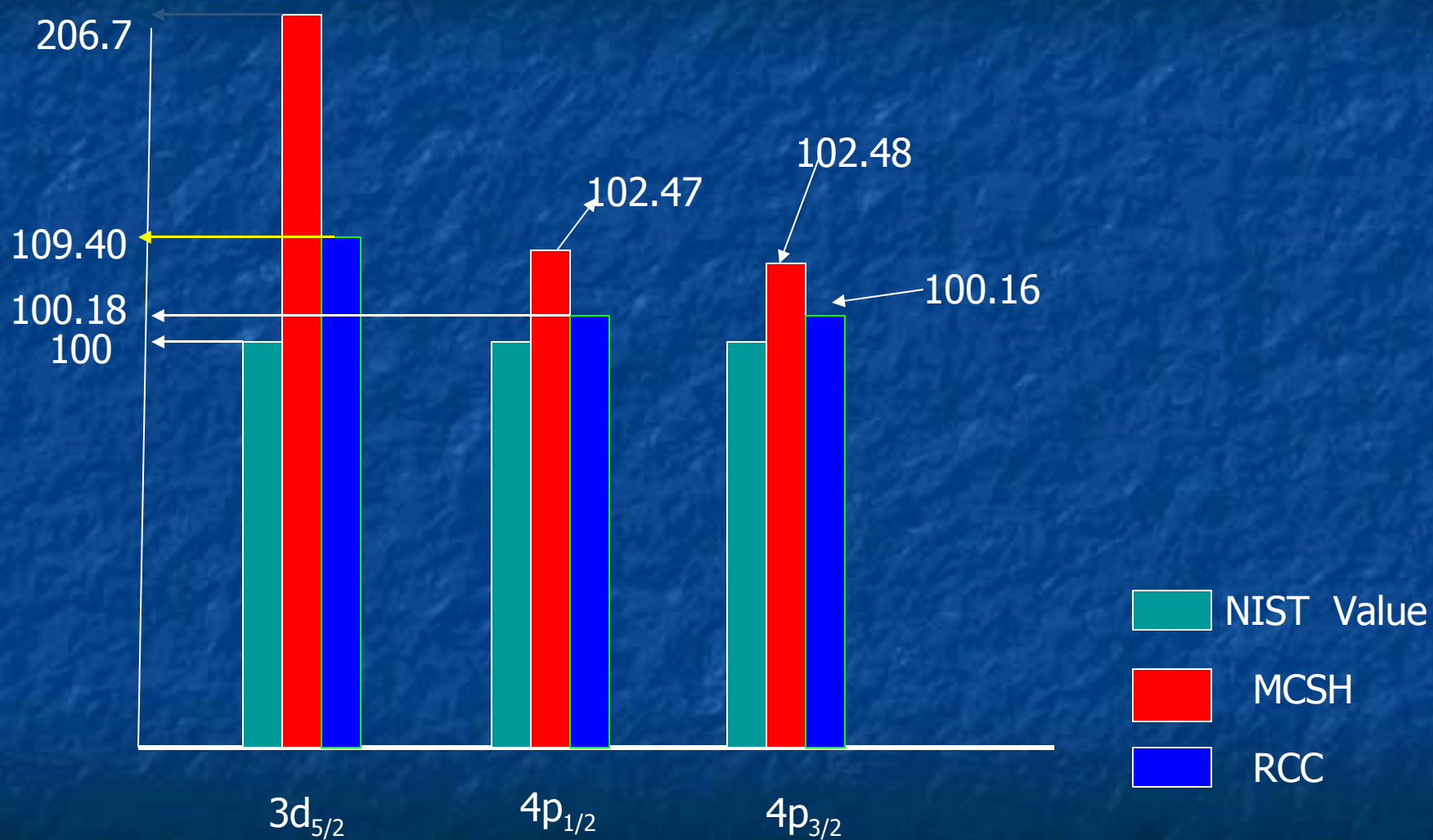
- Energy values are in excellent agreement with that of NIST value.

(In cm^{-1})

State	NIST	MCHF	RCC
$3d_{5/2}$	382.1	790.1	418.02
$4p_{1/2}$	127921.36	124749.38	127689.51
$4p_{3/2}$	128739.59	125539.49	128534.43
$5p_{1/2}$	230608.89	228714.51	231061.48

Results

Excitation Energies



%error with NIST energy value

Acknowledgment

- Dr. Sonjoy Majumder (IIT Madras)