Indirect Deexcitation Of $^{84}\text{Rb}$ in a Plasma Created at PHELIX
76Ge(11B,3n) 84Rb

γ: E=218.58 keV

Phelix

γ detector

The Final Experiment?

CEA-CENBG-GSI Collaboration

Gilbert GOSSELIN    San Francisco 2014
The Preliminary Experiment

CEA-CENBG-GSI Collaboration

84Rb

Phelix

Bragg Cristal
NEET Evaluation

- Nuclear Transition Energy: 3.05 keV now 3.50 keV
- Requires precise knowledge of atomic transition energy

MCDF (Multi-Configuration Dirac-Fock)

- Hamiltonian diagonalization for each J
- Precise atomic energies $\frac{\Delta E}{E} \approx 10^{-3}$
- Very Long Calculation Times
- Not the best way to get a spectrum
- Is probably best to get line energies for NEET calculations
Spectrum Evaluation

Spectrum

\[ S(E) = \sum_Q P_Q \sum_i P_i \frac{\Gamma}{(E - \Delta E_i)^2 + \frac{\Gamma^2}{4}} \]

Configuration Probability : Grand Canonical Partition Function

\[ P_Q P_i = \frac{(2j_i + 1)e^{-\frac{E_i}{kT}-Q\eta}}{\sum_k (2j_k + 1)e^{-\frac{E_k}{kT}-Q\eta}} \]

\[ \eta : \text{reduced chemical potential} \]
# Configuration Interaction

<table>
<thead>
<tr>
<th>Configuration Interaction (CI)</th>
<th>With</th>
<th>Without</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Definition</strong></td>
<td>$(n,l)$ (not j)</td>
<td>$(n,l,j)$</td>
</tr>
<tr>
<td></td>
<td>$(1s)^2 (2s)^1 (4p)^1 \rightarrow (1s)^2 (2s)^2$</td>
<td>$(1s_{1/2})^2 (2s_{1/2})^1 (4p_{3/2})^1 \rightarrow (1s_{1/2})^2 (2s_{1/2})^2$</td>
</tr>
</tbody>
</table>
| **Calculation Time**         | Long (very long…) | Long (much less so…)
| **Configuration Number**     | Not so Huge | Huge |
| **Precision**                | Even Better | Quite Good |
## Spectrum Evaluation

### Configuration Numbers

- Electrons from n=1 to n=6
- Transitions: n=3,4,5,6 → n=2
- Initial Configurations: 1s filled

<table>
<thead>
<tr>
<th>Charge State</th>
<th>With CI (All Transitions)</th>
<th>Without CI (3s&lt;sub&gt;1/2&lt;/sub&gt; to 2p&lt;sub&gt;1/2&lt;/sub&gt; only)</th>
</tr>
</thead>
<tbody>
<tr>
<td>34+</td>
<td>19</td>
<td>1</td>
</tr>
<tr>
<td>33+</td>
<td>33</td>
<td>559</td>
</tr>
<tr>
<td>32+</td>
<td>6,741</td>
<td>559</td>
</tr>
<tr>
<td>31+</td>
<td>32,699</td>
<td>6,741</td>
</tr>
<tr>
<td>30+</td>
<td>127,956</td>
<td>57,520</td>
</tr>
<tr>
<td>29+</td>
<td>444,310</td>
<td>418,359</td>
</tr>
<tr>
<td>28+</td>
<td>1,395,835</td>
<td>2,591,331</td>
</tr>
<tr>
<td>27+</td>
<td>4,026,185</td>
<td>14,049,302</td>
</tr>
<tr>
<td>26+</td>
<td>68,016,688</td>
<td></td>
</tr>
</tbody>
</table>

Configuration Selection is mandatory
Goal: Eliminate the less probable configurations

Problem: Partition function cannot be evaluated yet

- Configurations probabilities are unknown

Configuration probability estimation: Bernoulli

- Sub-shells occupation from average atom model

\[ P_i \approx \prod_k C_{D_k}^{n_k} (p_k)^{n_k} (1 - p_k)^{D_k - n_k} \]

Configurations are ordered by decreasing probability

\[ P_1 > P_2 > P_3 > ... > P_N \]

Configurations selection under cumulated \( P_{\text{threshold}} \)

\[ \sum_{k=1}^{N_{\text{sel}}} P_k \geq P_{\text{threshold}} \]
Configuration Selection

\( T_e = 270 \text{ eV} \)
## Configuration Numbers

Initial Configurations: 1s full, electrons from n=1 to n=6

<table>
<thead>
<tr>
<th>Charge State</th>
<th>With CI (All Transitions)</th>
<th>Without CI (3s(<em>{1/2}) to 2p(</em>{1/2}) only)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>With CI</td>
<td>Without CI</td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>Selected (99,9 %)</td>
</tr>
<tr>
<td>34+</td>
<td>19</td>
<td>19</td>
</tr>
<tr>
<td>33+</td>
<td>190</td>
<td>180</td>
</tr>
<tr>
<td>32+</td>
<td>1,325</td>
<td>397</td>
</tr>
<tr>
<td>31+</td>
<td>7,220</td>
<td>869</td>
</tr>
<tr>
<td>30+</td>
<td>32,699</td>
<td>1,529</td>
</tr>
<tr>
<td>29+</td>
<td>127,956</td>
<td>1,956</td>
</tr>
<tr>
<td>28+</td>
<td>444,310</td>
<td>1,704</td>
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<tr>
<td>27+</td>
<td>1,395,835</td>
<td>2,821</td>
</tr>
<tr>
<td>26+</td>
<td>4,026,185</td>
<td>5,225</td>
</tr>
</tbody>
</table>
Bernoulli vs Partition Function

$T_e = 270 \text{ eV}$

Fundamental Configurations
Charge States under Non LTE Conditions

**FlyCHK**

![Graph showing charge states vs. electronic temperature](image)

- Ionic Fraction
  - $Q$ | $P_Q$
  - $26^+$ | 8.48 %
  - $27^+$ | 39.5 %
  - $28^+$ | 39.1 %
  - $29^+$ | 11.0 %
  - $30^+$ | 1.05 %

From AVERROES & FlyCHK

\[
T_z = 270 \text{ eV} \quad T_{\text{HETL}} = 1.4 \text{ keV}
\]
Experimental Spectrum vs MCDF Spectrum (no CI)

D. Denis-Petit et al., JQSRT 148 (2014) 70-89
Experimental Spectrum vs MCDF Spectrum (no Cl)

D. Denis-Petit et al., JQSRT 148 (2014) 70-89
Most lines have been identified

- Energy, initial configuration, angular momentum
- More than 50 new lines previously unidentified

Charge states distribution

- Ionization temperature model is fine

Line intensities are globally good within a factor of 2 or 3

- Exception around 7 Å
Spectrum with CI vs without CI

\[ T_e = 270 \text{ eV} \]
Spectrum with CI vs without CI

$T_e = 270 \text{ eV}$
Alternative Atomic Physics Models

- AVERROES
  - Superconfigurations approach
  - Native non-LTE
  - Partial LTE within superconfigurations

- SCO-RCG
  - Combines statistical and detailed approach
  - SOSA (Spin Orbit Split Array)
  - Transition arrays subdivided into sub arrays (SO effect)
Spectrum

AVERROES and SCO-RCG: Courtesy of F. Gilleron & J. C. Pain

\[ T_e = 270 \text{ eV} \]
What about the new transition energy?

$T_e = 270 \text{ eV}$
Conclusion & Perspectives

- Experimental spectrum is well restituted
  - MCDF calculations with or without CI
  - Very time consuming
  - Agreement with AVERROES calculations
- Rubidium 84 is probably not the best candidate
  - $n=4,5,6 \rightarrow n=2$ nearly impossible with $\Delta E=3,50$ keV
  - Higher transition energy than expected
  - Optimum Charge state for NEET is now $30^+/32^+$
- Future NEET calculations
  - Will require MCDF with CI
  - Alternate ADAM model (see next talk with M. Comet)
Thank you for your attention

Questions are welcome