Analysis of theoretical calculations of rotationally inelastic collisions of He with NaK and Ar with NaK: rotational constants and cross sections in context of the vector model

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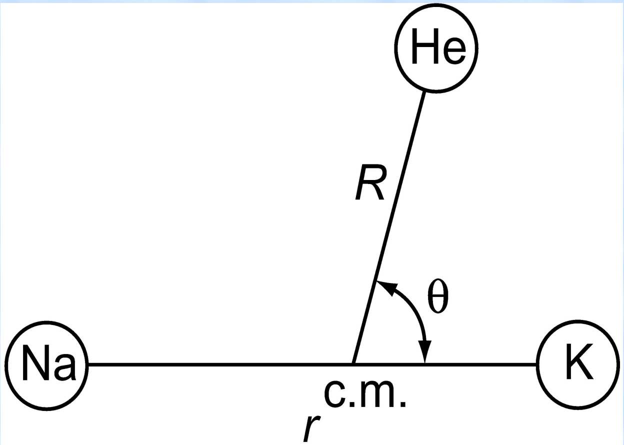
Background

- Experiment and theory
  - Rotationally inelastic collision
- Cross section – measure of likelihood of collision



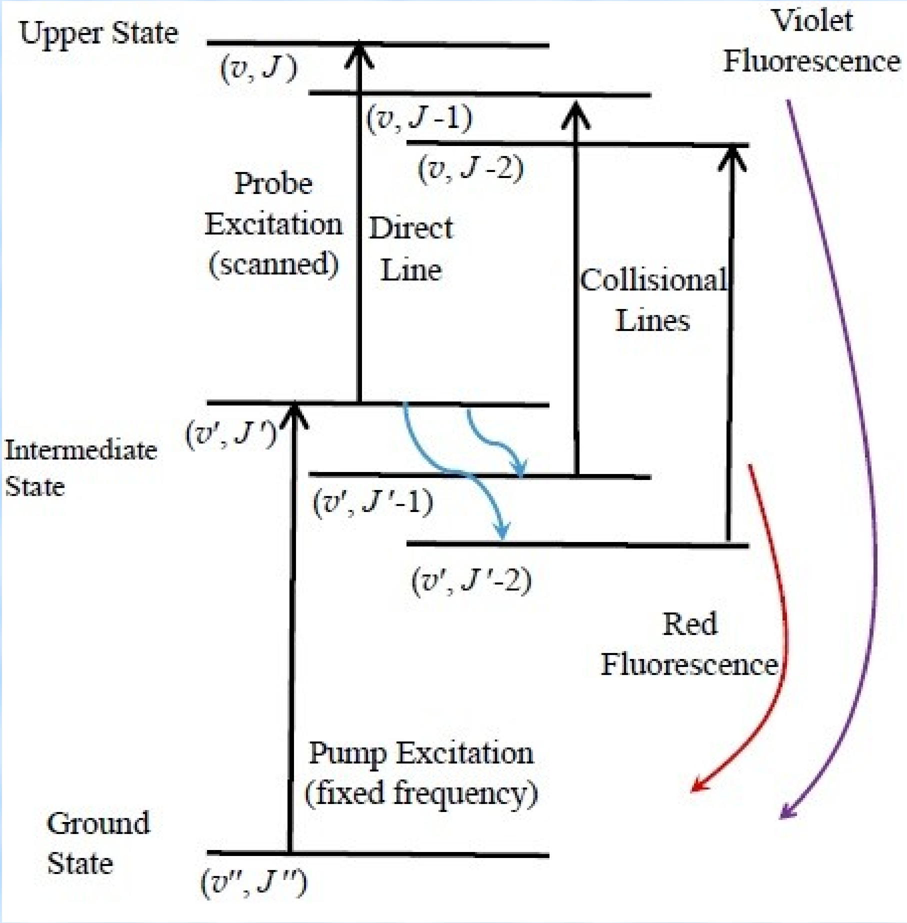
$$He + NaK(j,m) \rightarrow He + NaK(j',m')$$
$$Ar + NaK(j,m) \rightarrow Ar + NaK(j',m')$$

Experimental background

- Experimental setup
  - Oven with NaK, He, or NaK, Ar
    - Na, K, Na_2, K_2
  - Pump laser
    - Excite the system to a particular state
  - Probe laser
    - Excite the excited state for a particular energy

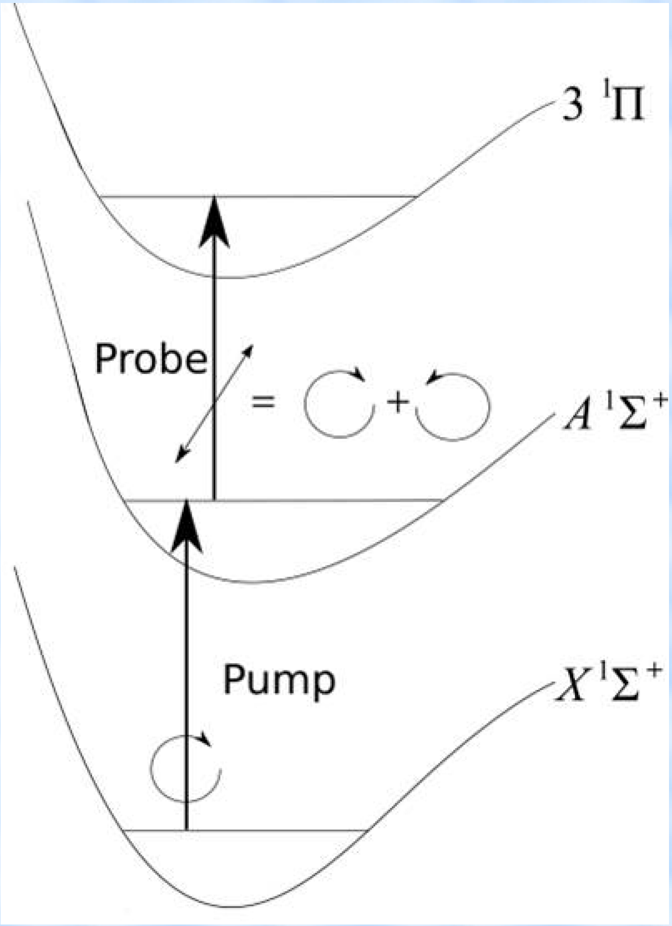
Experimental background

- Measure transitions from excited states to ground state



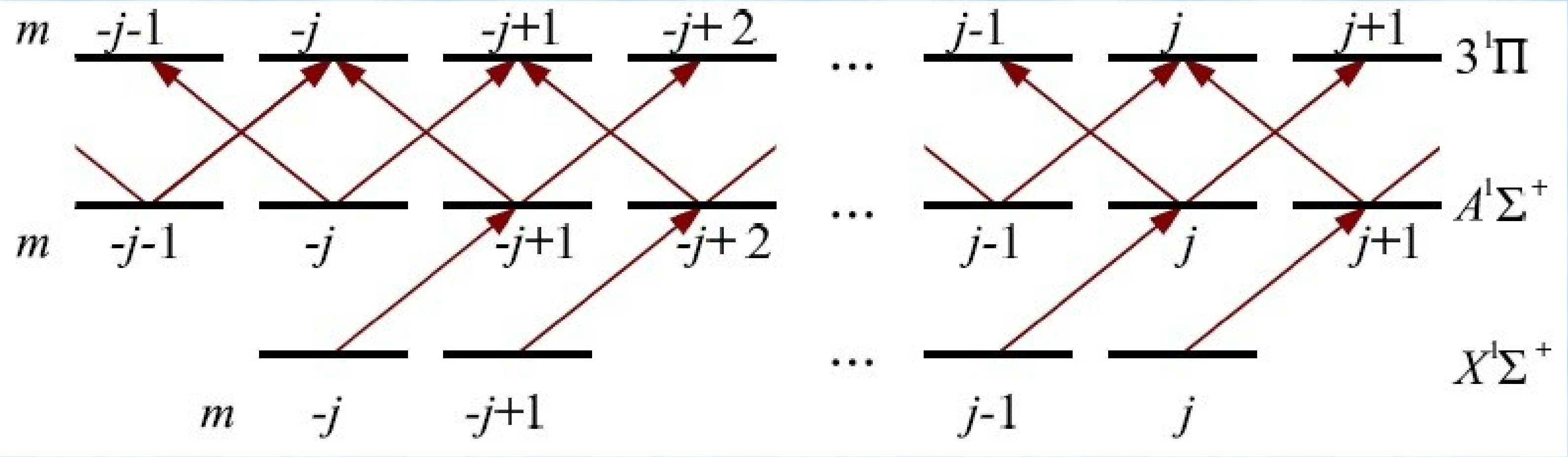
Experimental background

- Alignment and orientation
  - Rotationally excited states



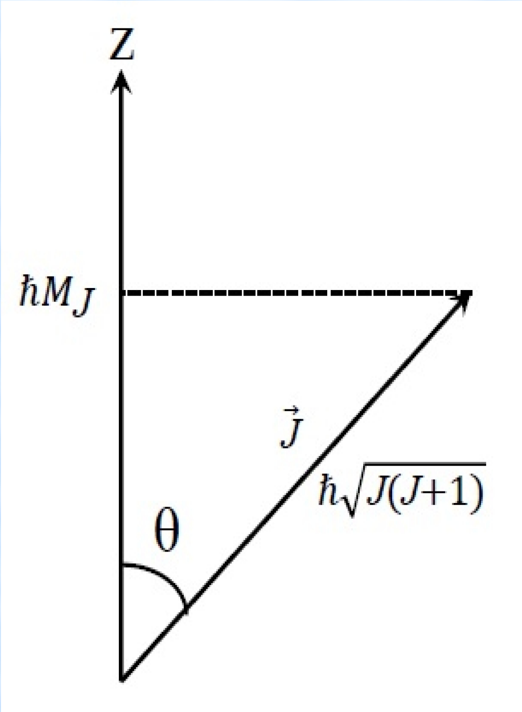
Experimental background

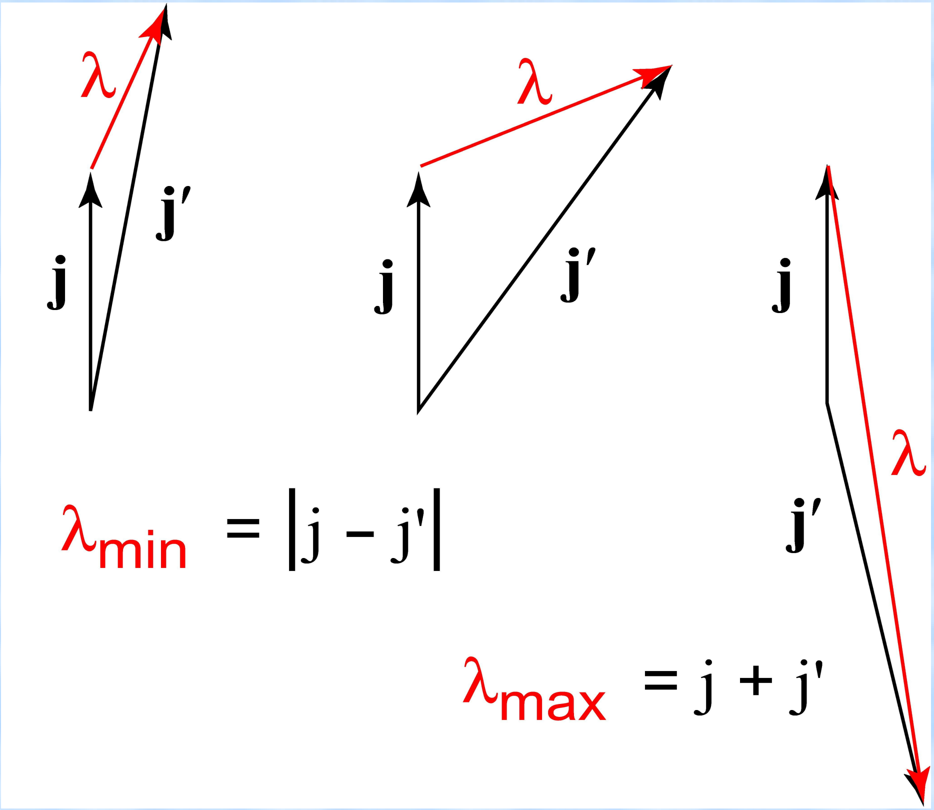
- Rotationally excited states
  - Controls average population, alignment, and orientation prior to collisions



Theoretical background

- Vector model for angular momentum
  - j,m → j',m'





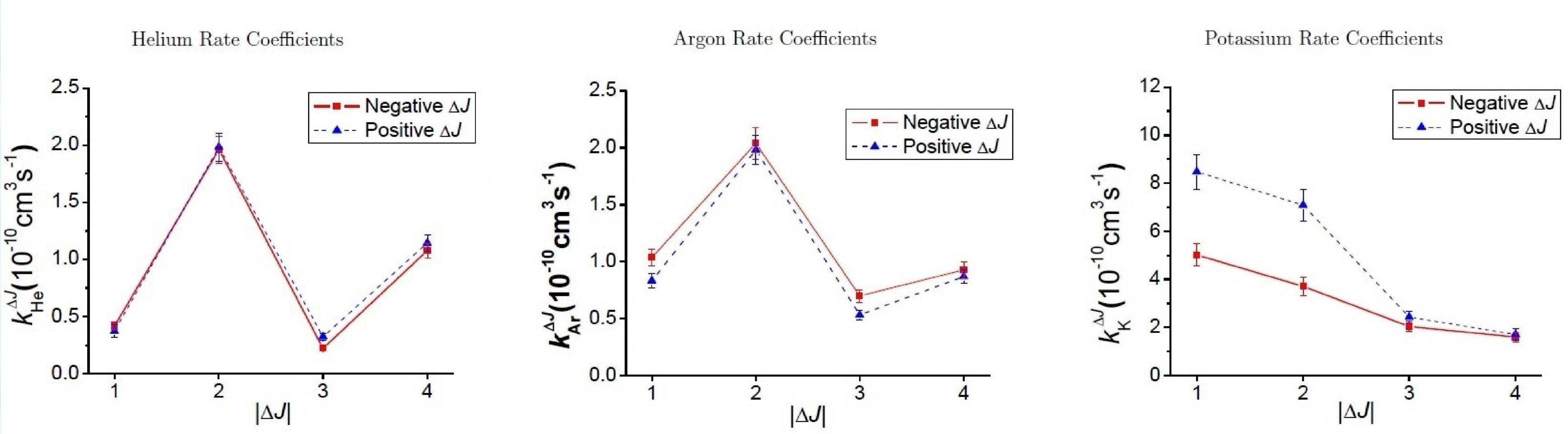
Theoretical background

- Quantum mechanical (QM) model
  - Cross section parameters: j, j', m, m', λ, k_j, B(j,j',λ)
  - Sum over λ
- Semiclassical (SC) model
  - Cross section parameters: j, j', α, k_j, B(j,j',cos(α))
  - Integrate over α

$$\lambda(\lambda+1)=j(j+1)+j'(j'+1)-2\sqrt{j(j+1)\,j'(j'+1)}\cos(\alpha)$$

Past results

- Propensity for Δj to be even
  - Strict selection rule for homonuclear molecules
- As $\bar{j}$ increases, λ decreases
  - Larger $\bar{j}$ corresponds to less change in orientation and alignment where $\bar{j}=(j+j')/2$



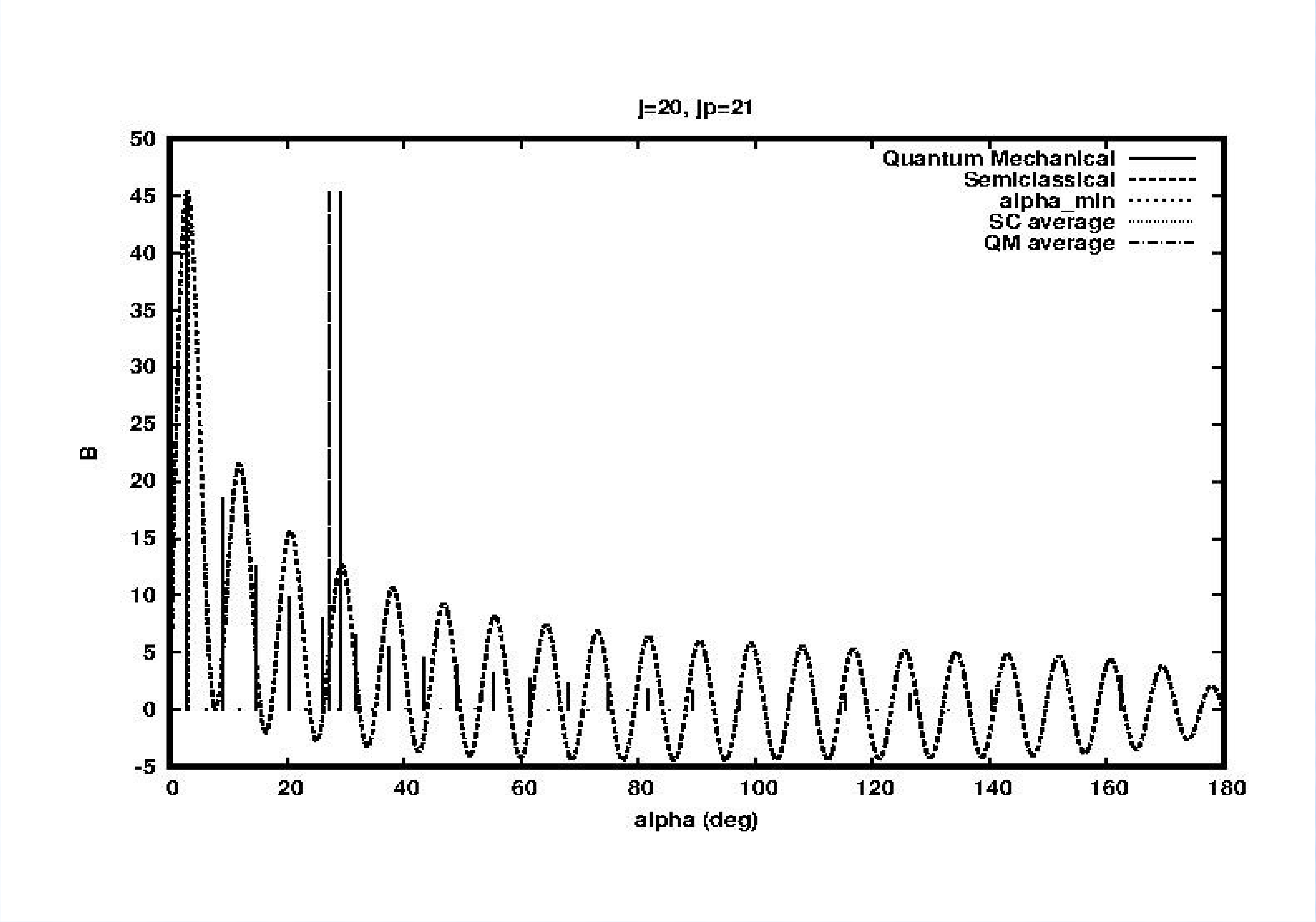
Data analysis

- Comparisons
  - quantum mechanical and semiclassical models
  - Argon, helium
- Focus
  - B values, tipping angle
  - Cross section values

$B(j,j',\lambda)$ vs $B(j,j',\cos(\alpha))$

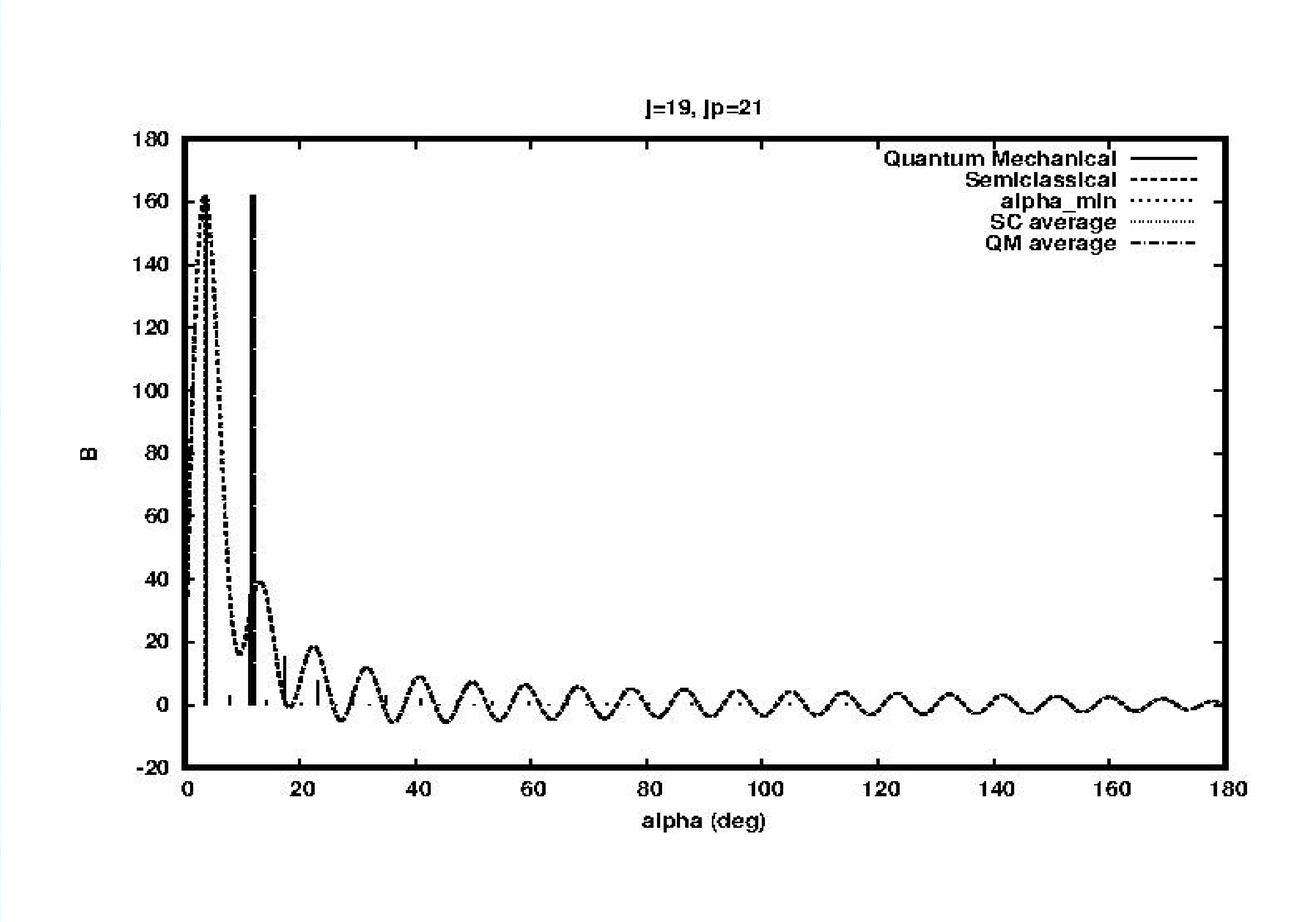
- Plotted $B(j,j',\lambda)*(2\lambda+1)$ and $B(j,j',\cos(\alpha))*(\sin(\alpha))$ vs θ
- Angular distribution
- Larger average tipping angle
  - He for odd Δj and as $\bar{j}$ increases
  - Ar as $\bar{j}$ increases

Helium, Δj=1



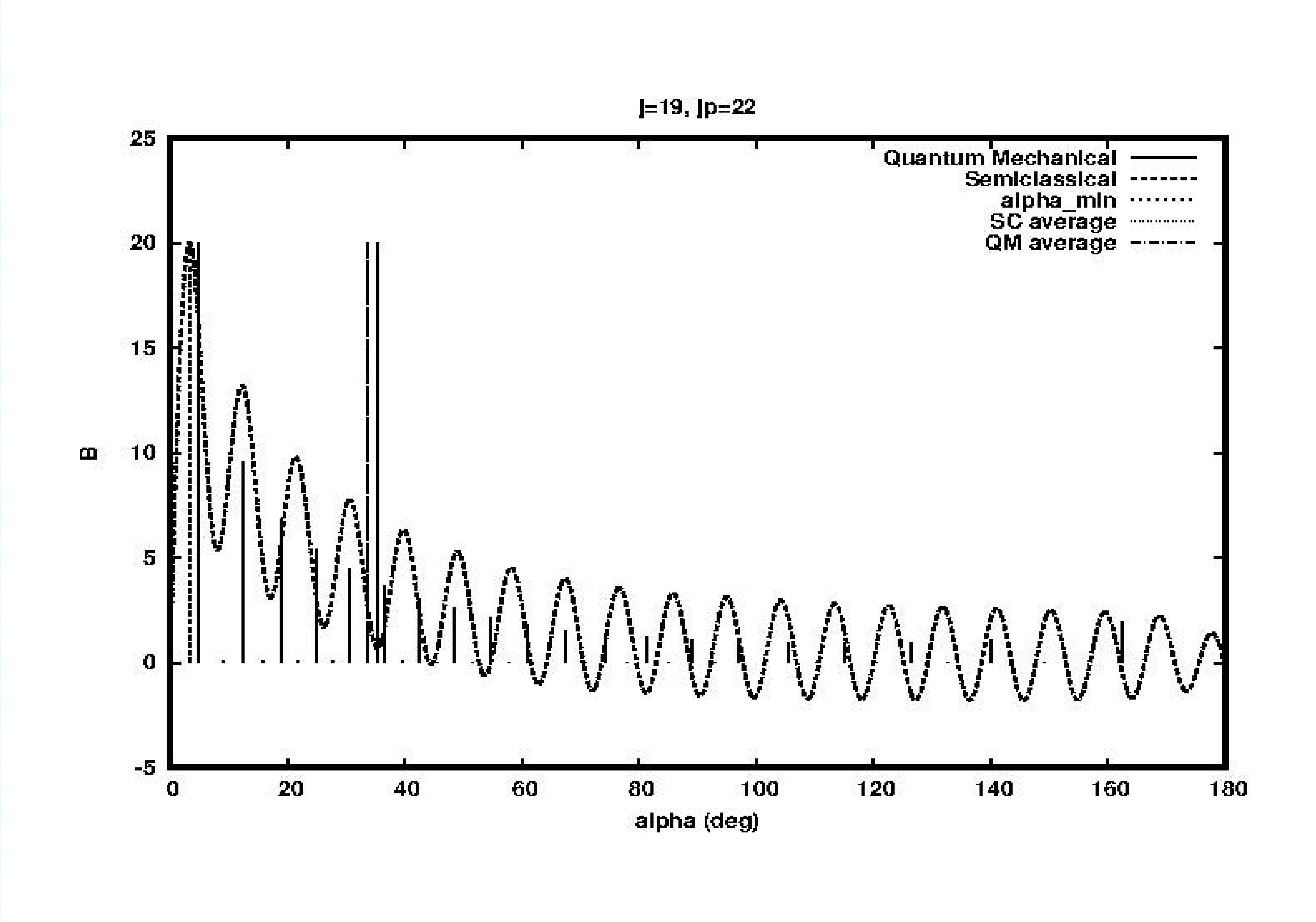
j=20, jp=21
Quantum Mechanical
Semiclassical
alpha_min
SC average
QM average
B
alpha (deg)
50
45
40
35
30
25
20
15
10
5
0
-5
0
20
40
60
80
100
120
140
160
180

Helium, Δj=2



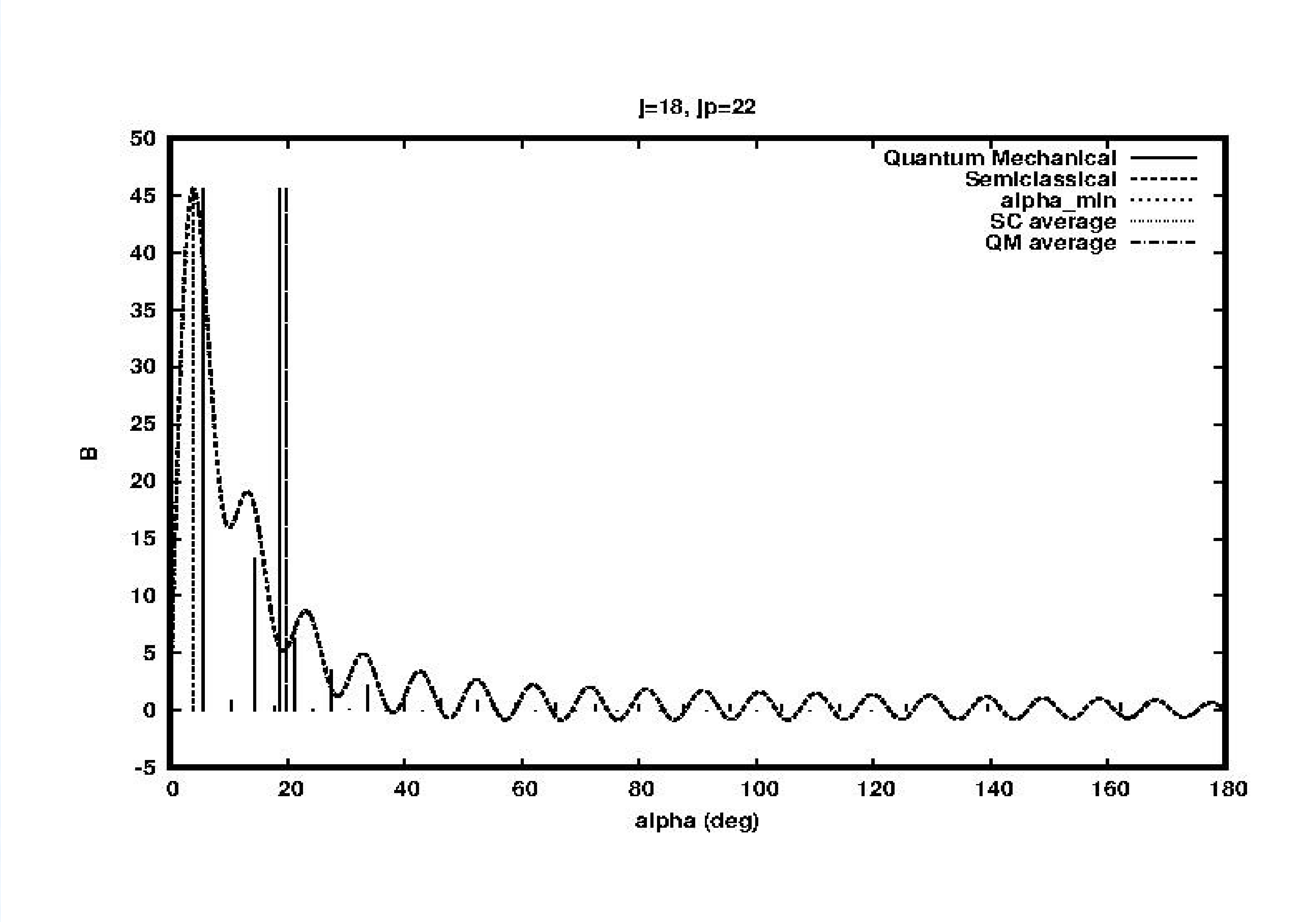
j=19, jp=21
Quantum Mechanical
Semiclassical
alpha_min
SC average
QM average
B
alpha (deg)
180
160
140
120
100
80
60
40
20
0
-20
0
20
40
60
80
100
120
140
160
180

Helium, Δj=3



j=19, jp=22
Quantum Mechanical
Semiclassical
alpha_min
SC average
QM average
B
alpha (deg)
25
20
15
10
5
0
-5
0
20
40
60
80
100
120
140
160
180

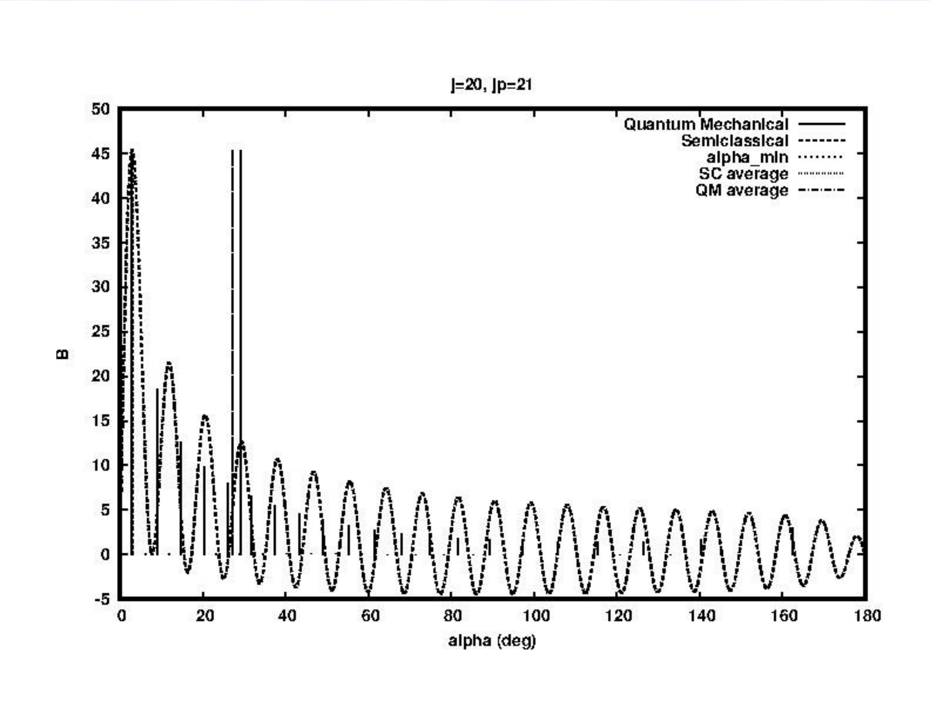
Helium, Δj=4

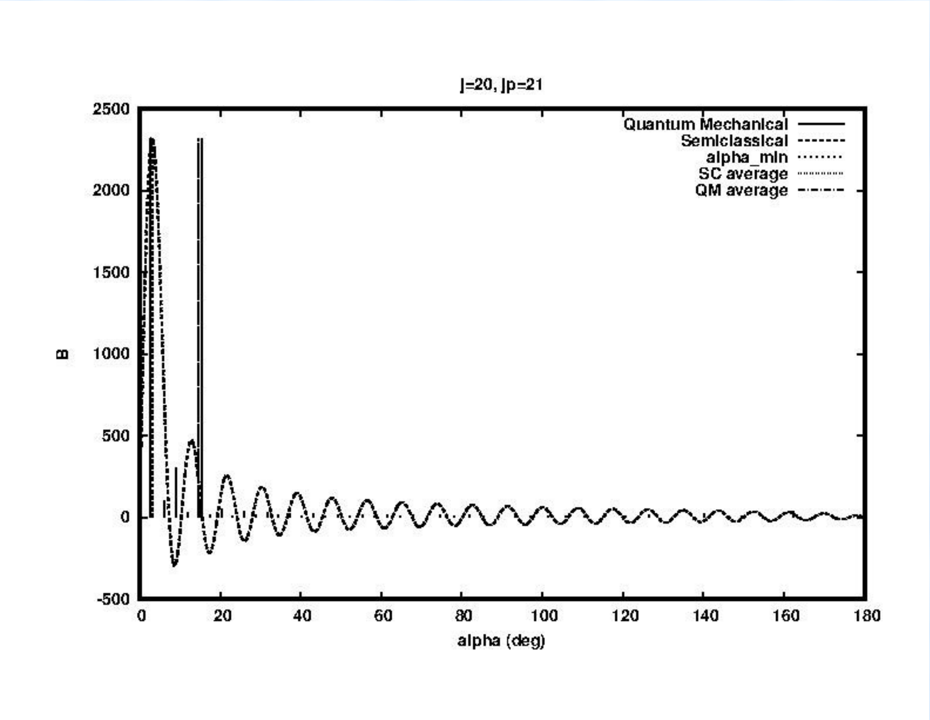

j=18, jp=22
Quantum Mechanical
Semiclassical
alpha_min
SC average
QM average
B
alpha (deg)
50
45
40
35
30
25
20
15
10
5
0
-5
0
20
40
60
80
100
120
140
160
180

Δj=1

Helium

Argon

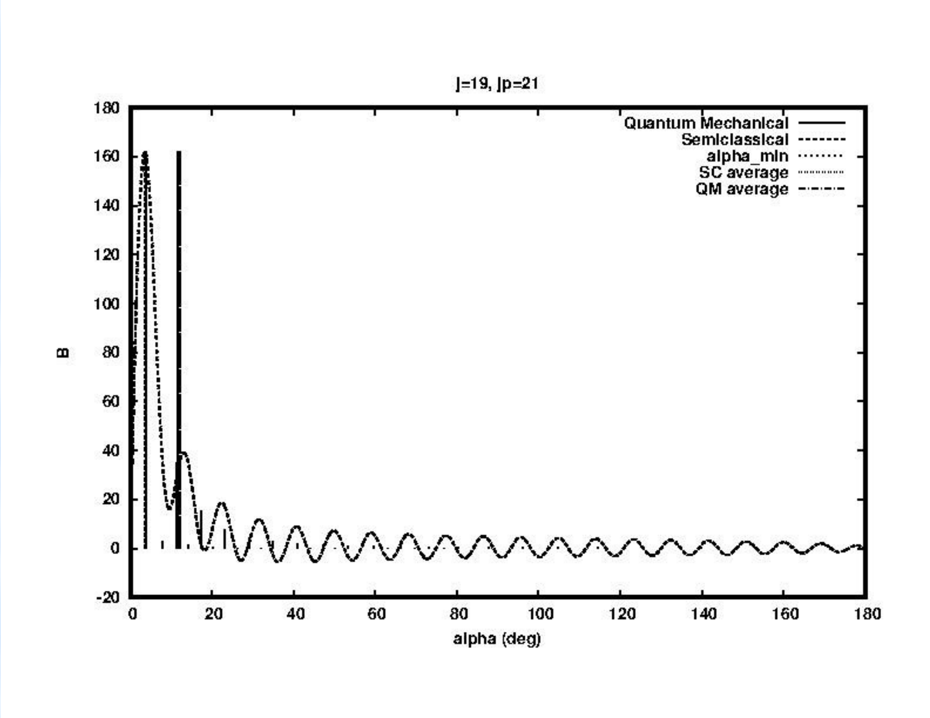


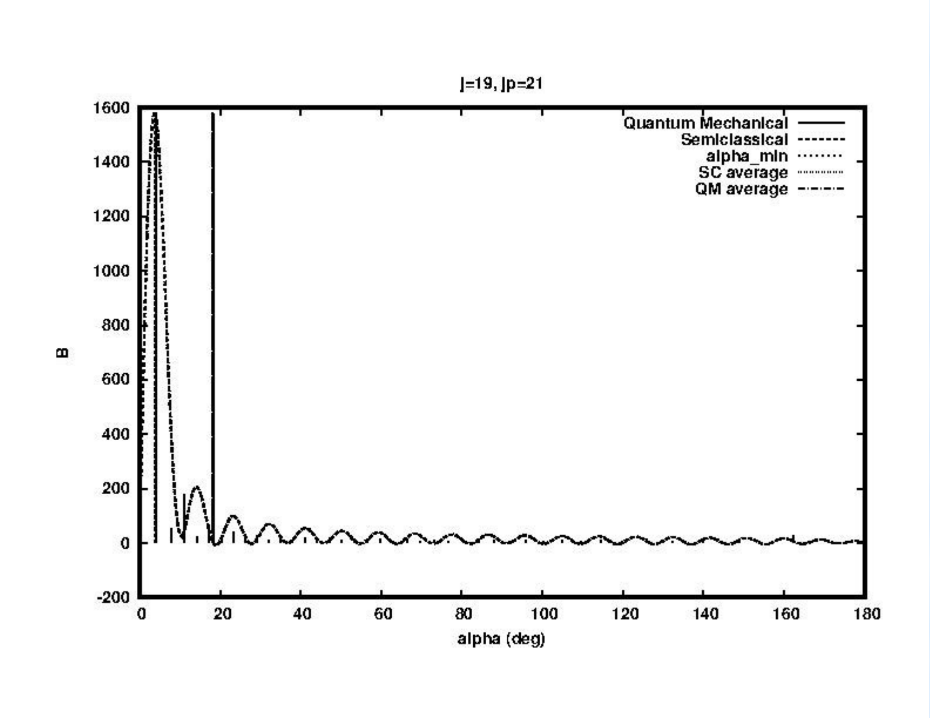


Δj=2

Helium

Argon

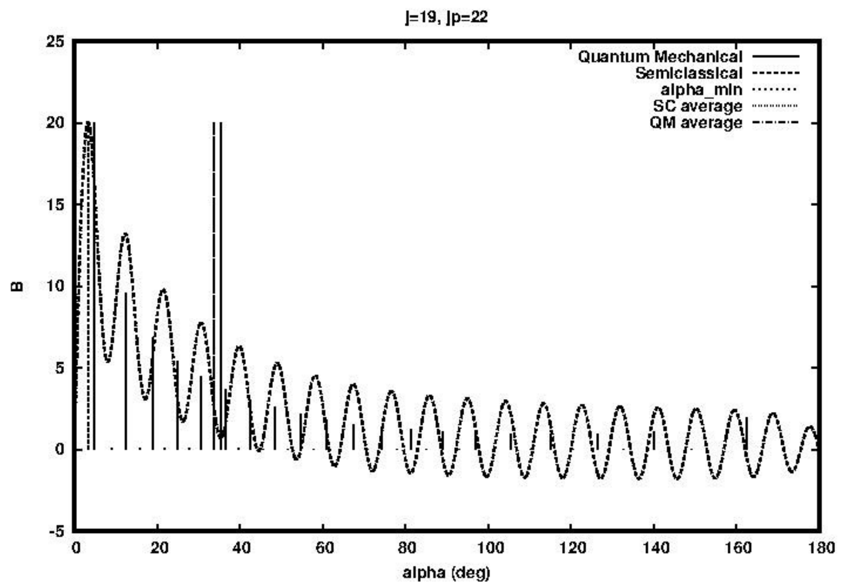


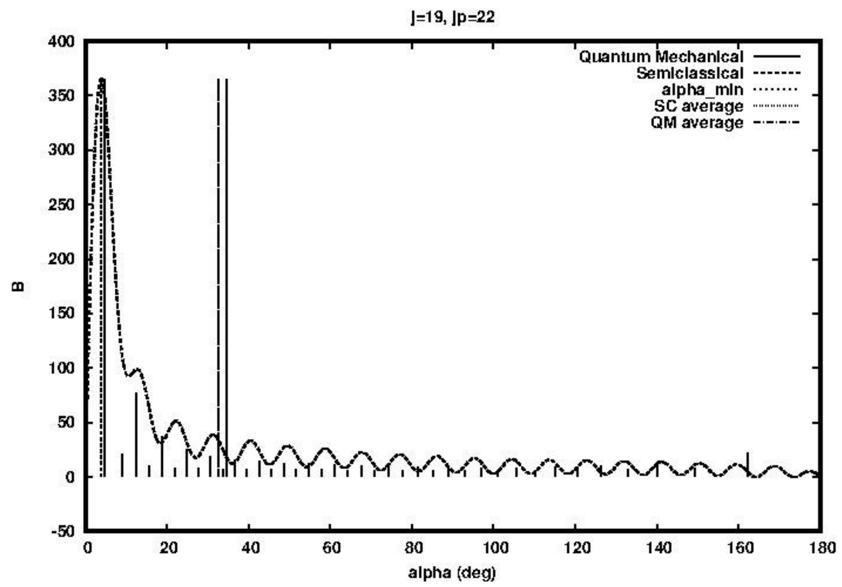


Δj=3

Helium

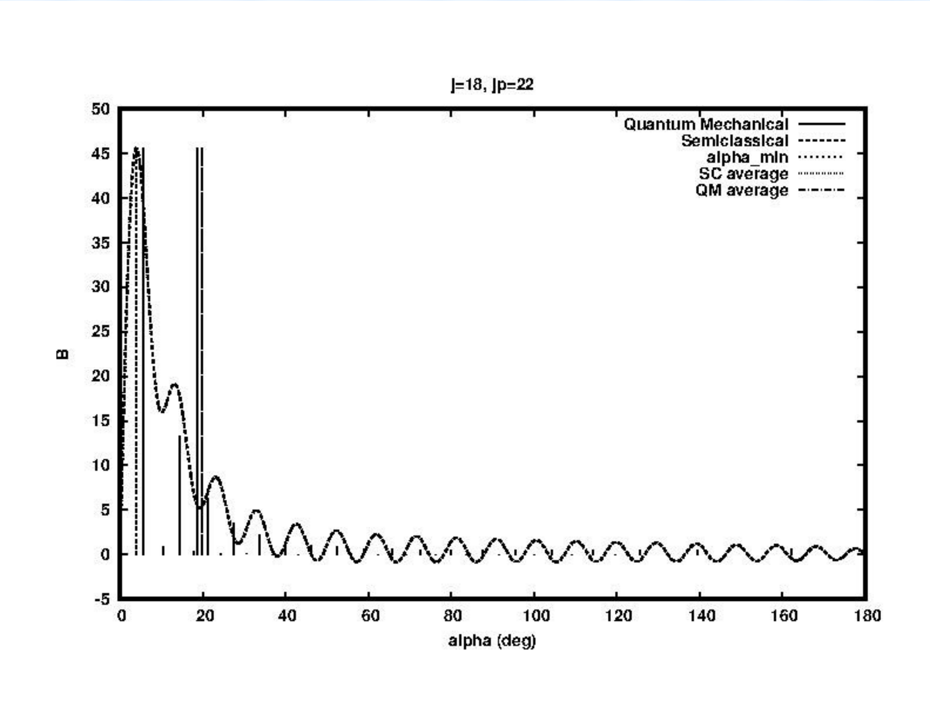
Argon



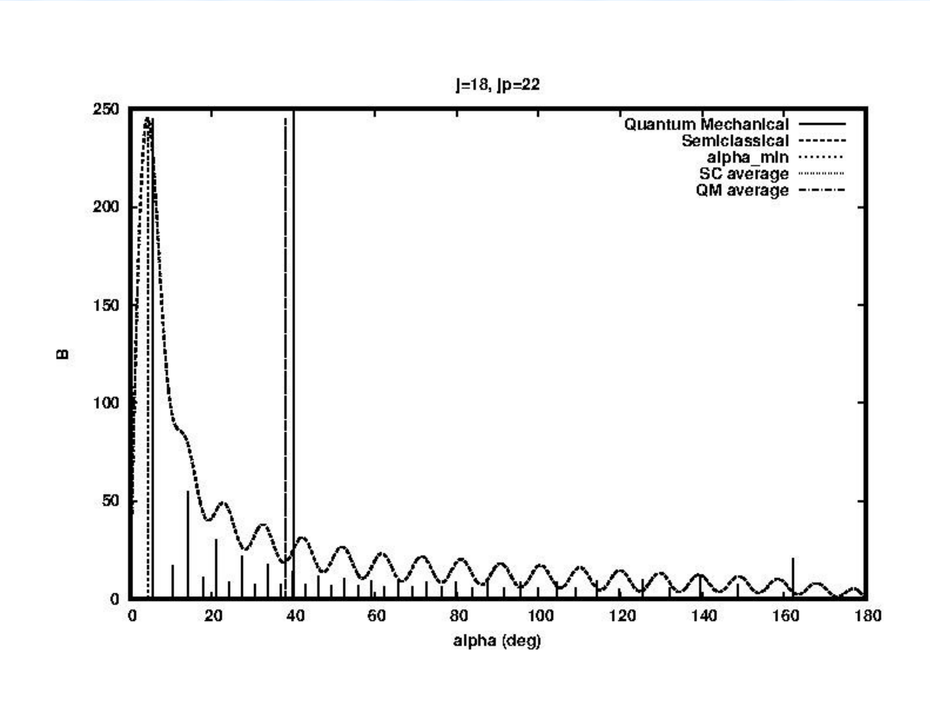


Δj=4

Helium



Argon



Trends in B

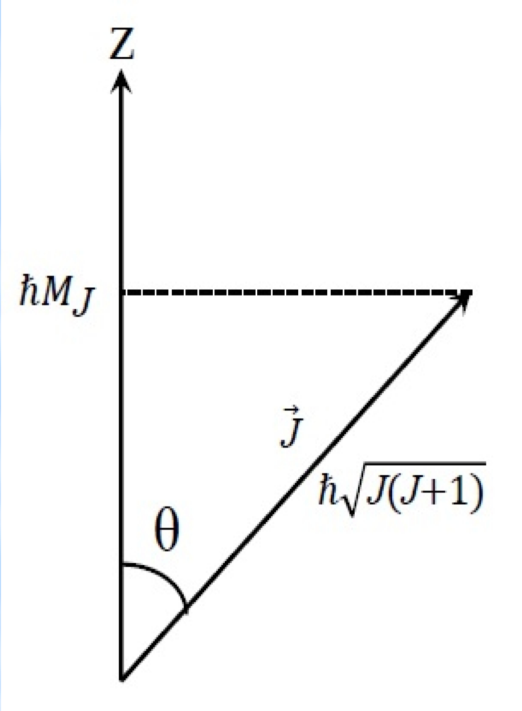
- Helium
  - Larger average tipping angle for odd Δj than even Δj
  - α is small for the more probable transitions
- Argon
  - Larger average tipping angle as Δj increases
  - No even/odd Δj propensities
- Comparison
  - Argon B values are larger
  - As $\bar{j}$ increases, $\langle\alpha\rangle$ decreases

Cross sections (σ)

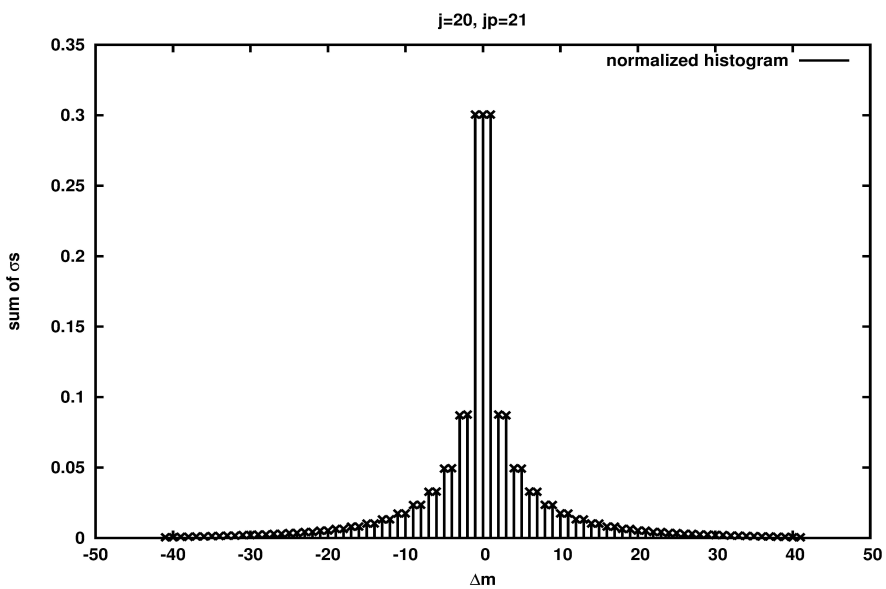
- $\sigma(jm \rightarrow j'm')$
  - Quantum mechanical: j, j', m, m', λ, k_j, B(j,j',λ)
  - Semiclassical: j, j', α, k_j, B(j,j',cos(α))
- Δθ

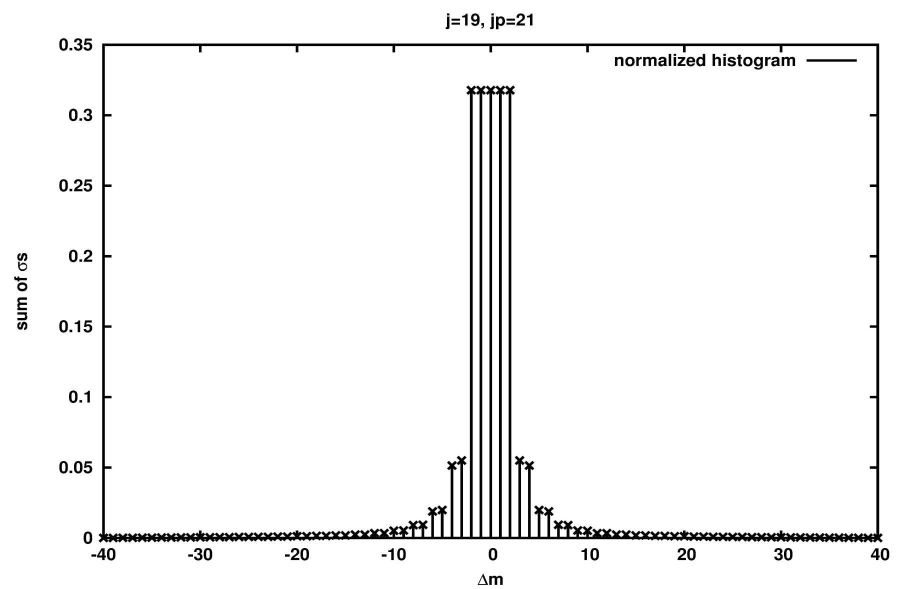
$$\cos(\theta) = \frac{m}{\sqrt{j(j+1)}}$$

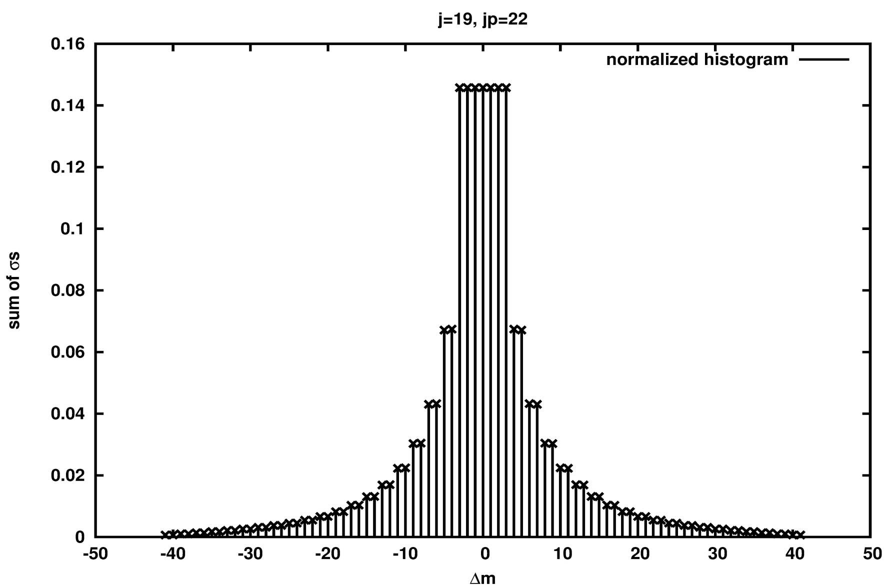
$$\Delta\theta = \cos^{-1}\left(\frac{m'}{\sqrt{j'(j'+1)}}\right) - \cos^{-1}\left(\frac{m}{\sqrt{j(j+1)}}\right)$$

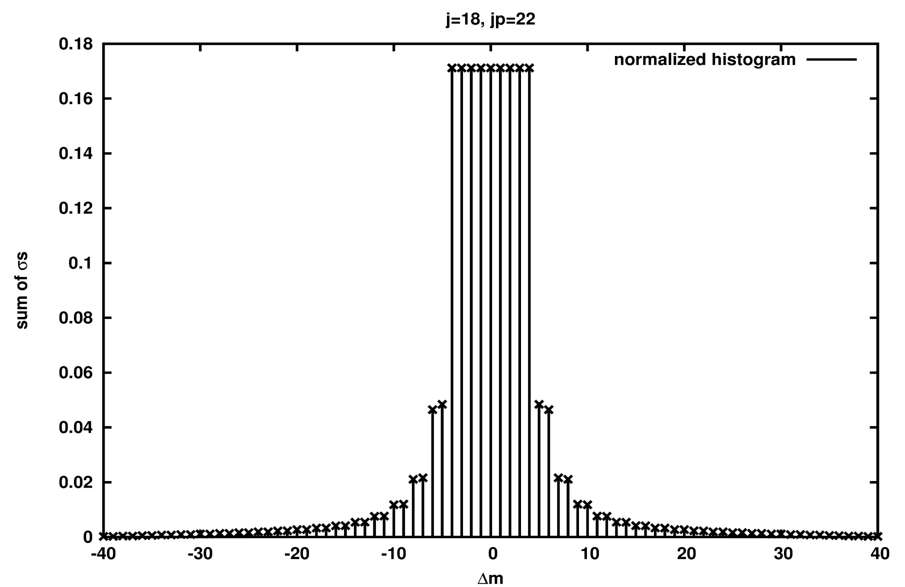


Grawert coefficients identity (QM)









Grawert coefficients identity

Cross sections:

$$\sigma(jm \rightarrow j'm') = \left(\frac{\pi}{k_j^2}\right) \sum_{\lambda=|j-j'|}^{j+j'} (2\lambda+1) \begin{pmatrix} j & j' & \lambda \\ -m & m' & m-m' \end{pmatrix}^2 B_\lambda(j,j') \quad (1)$$

$$\sigma(j \rightarrow j') = \sum_{m'=-j'}^{j'} \sigma(jm \rightarrow j'm') \quad (2)$$

$$\sigma(j \rightarrow j') = \left(\frac{\pi}{k_j^2}\right) \sum_{\lambda=|j-j'|}^{j+j'} (2\lambda+1) B_\lambda(j,j') \sum_{m'=-j'}^{j'} \begin{pmatrix} j & j' & \lambda \\ -m & m' & m-m' \end{pmatrix}^2 \quad (3)$$

Grawert coefficients:

$$\sum_{m_1} \sum_{m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{1}{2j_3+1} \delta_{j_3 j_3'} \delta_{m_3 m_3'} \quad (4)$$

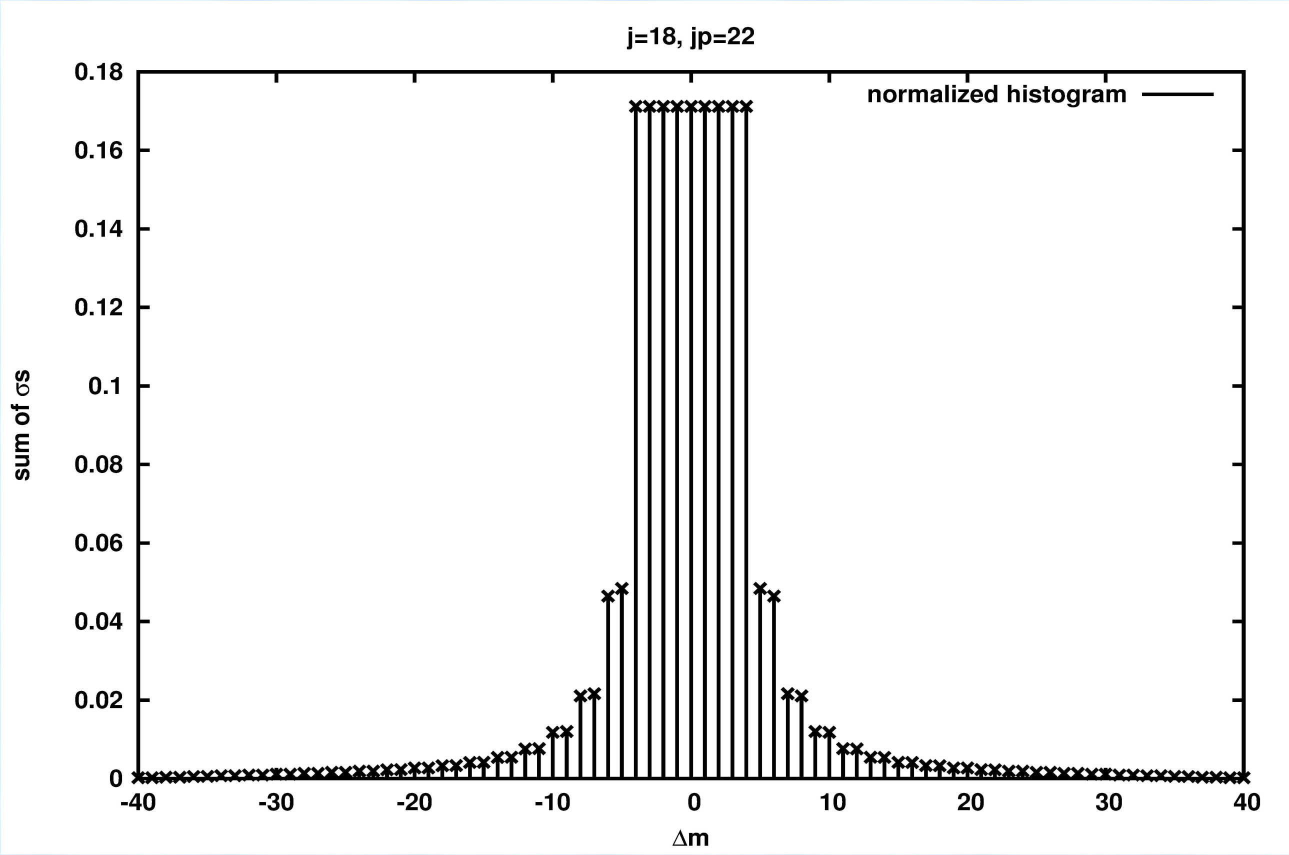
$$\sum_{m_1} \sum_{m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2 = \frac{1}{2j_3+1}, \text{ where } \left\{ \begin{matrix} j_3 = j_3' \\ m_3 = m_3' \end{matrix} \right\} \quad (5)$$

$$\sum_{m_1} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & m_1+\Delta m & \Delta m \end{pmatrix}^2 = \frac{1}{2j_3+1}, \text{ where } \left\{ \begin{matrix} m_1+m_2 = \Delta m \\ m_3 = \Delta m \end{matrix} \right\} \quad (6)$$

$$\sigma(j \rightarrow j') = \sum_{\lambda} f(j, j', \lambda) \frac{1}{2\lambda+1} \quad (7)$$

Thanks to Prof. Hickman for showing this mathematically

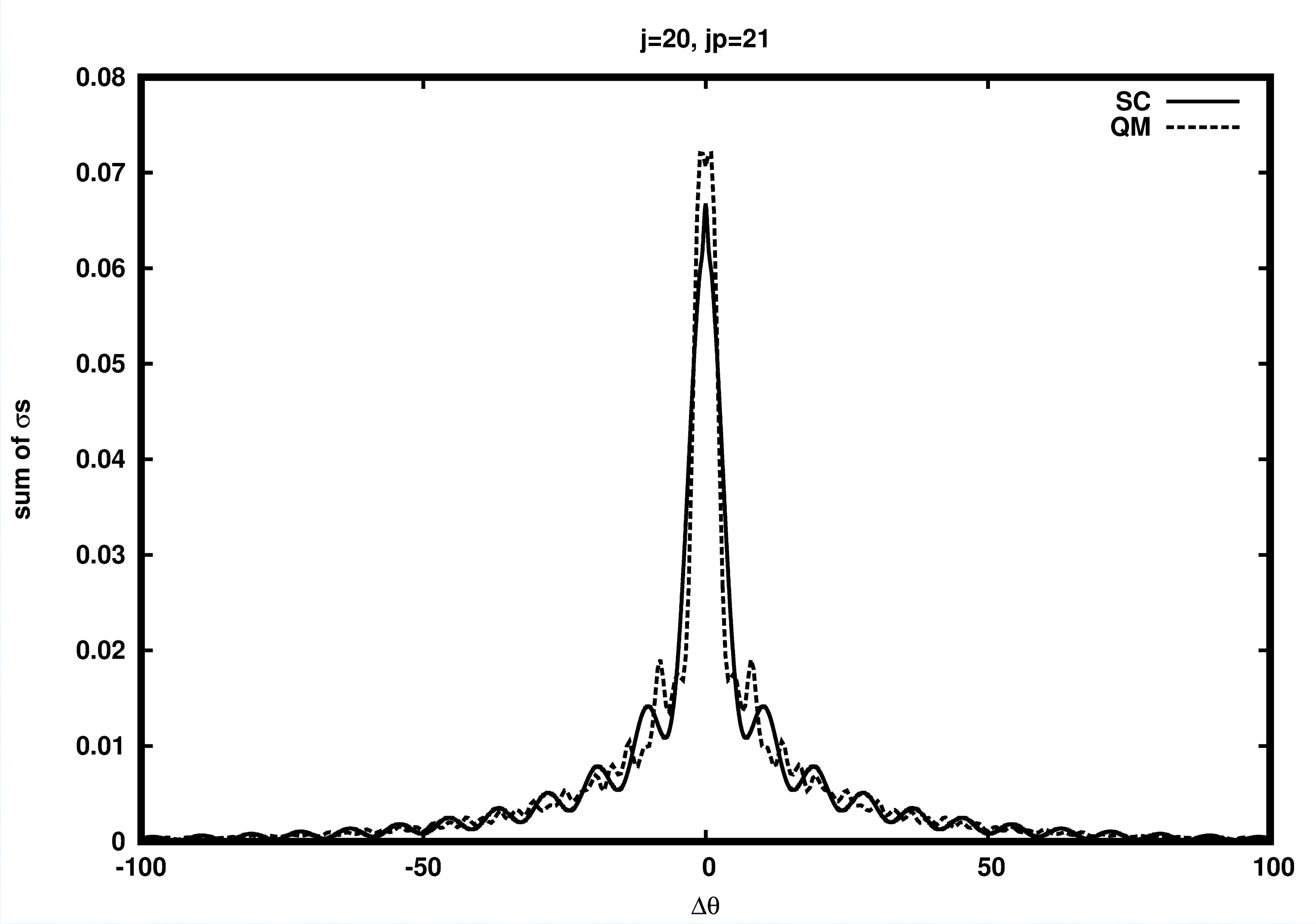
Helium, Δj=4
peak width = 2Δj+1



Methods for Δθ analysis

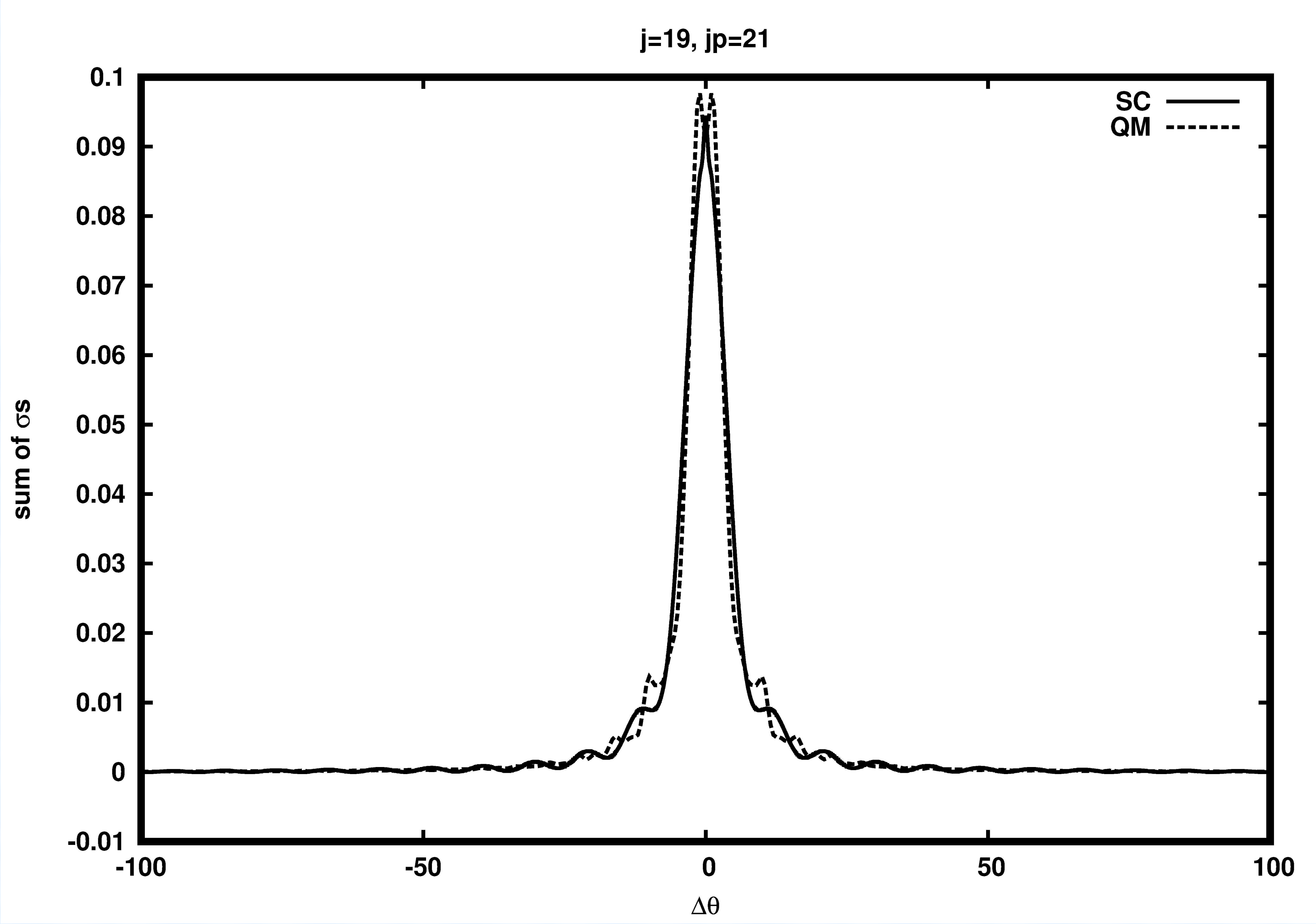
- Quantum mechanical model
  - Compute Δθ from j, j', m, m'
  - Create histogram angle bins
  - Smooth with Gaussian filter
- Numerically compute semiclassical model

Helium, Δj=1

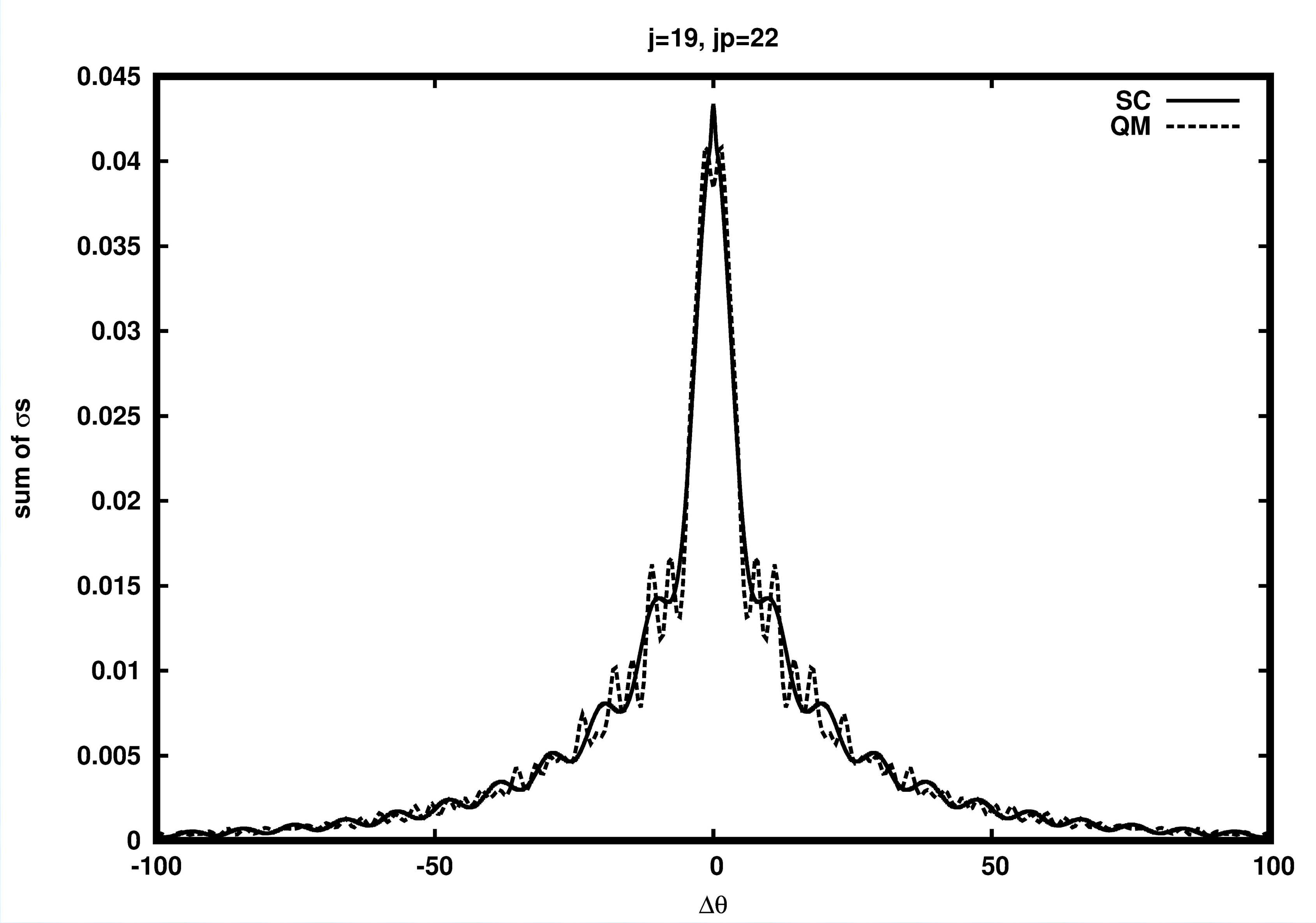


j=20, jp=21
SC
QM
sum of σs
Δθ
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-100
-50
0
50
100

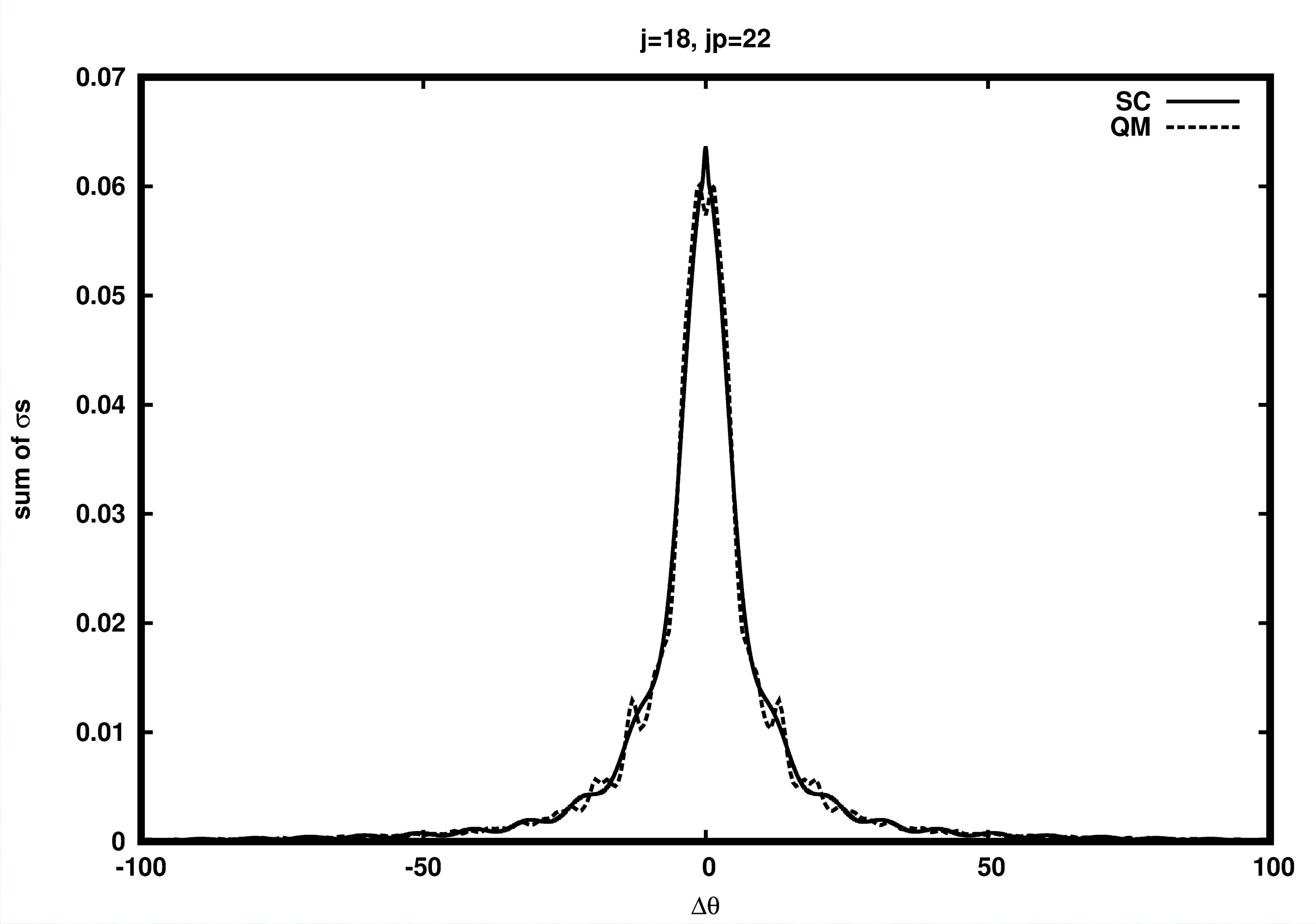
Helium, Δj=2


j=19, jp=21
SC
QM
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
sum of σs
-100
-50
0
50
100
Δθ

Helium, $\Delta j=3$



Helium, Δj=4

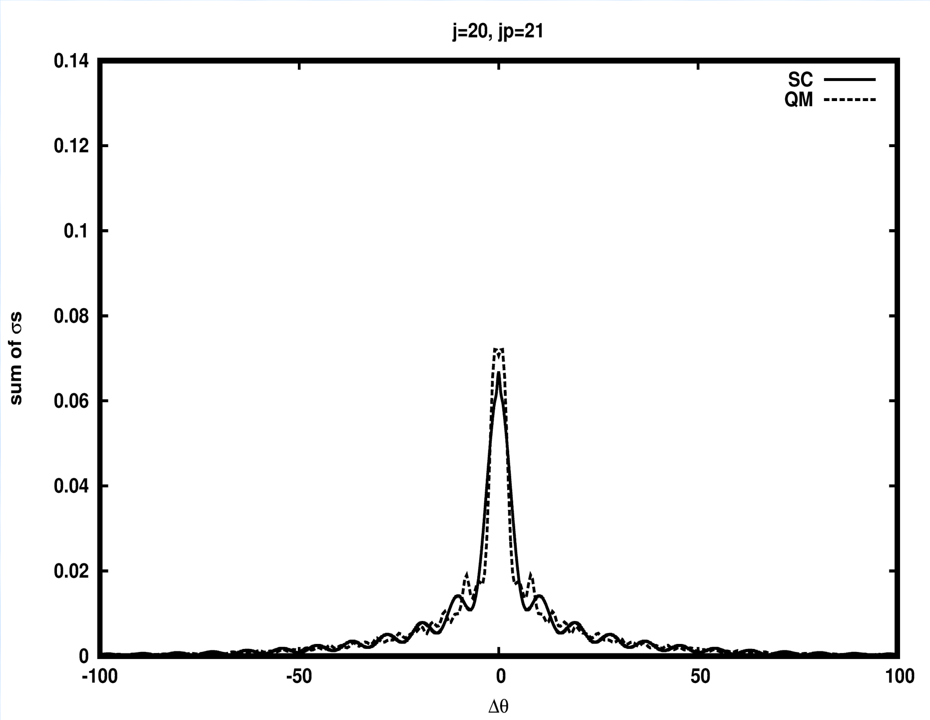


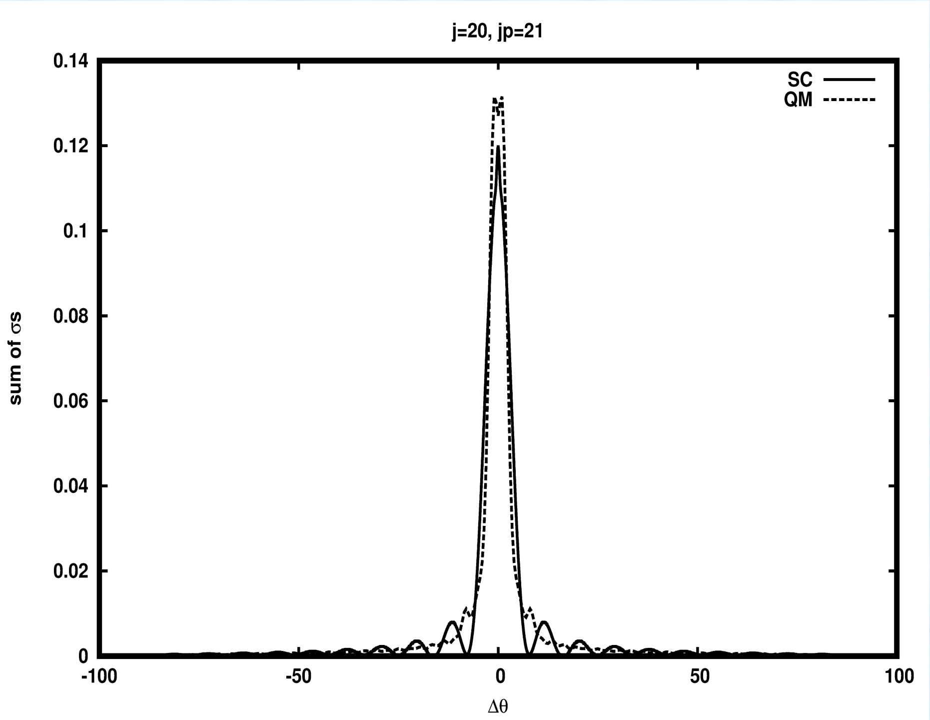
j=18, jp=22
SC
QM
sum of σs
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-100
-50
0
50
100
Δθ

Δj=1

Helium

Argon

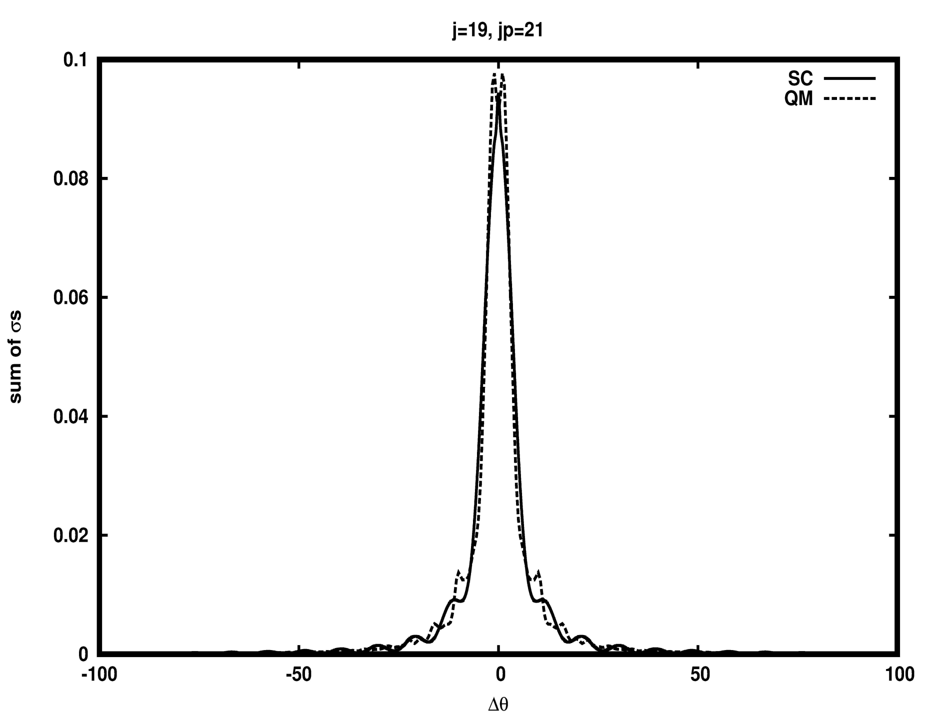


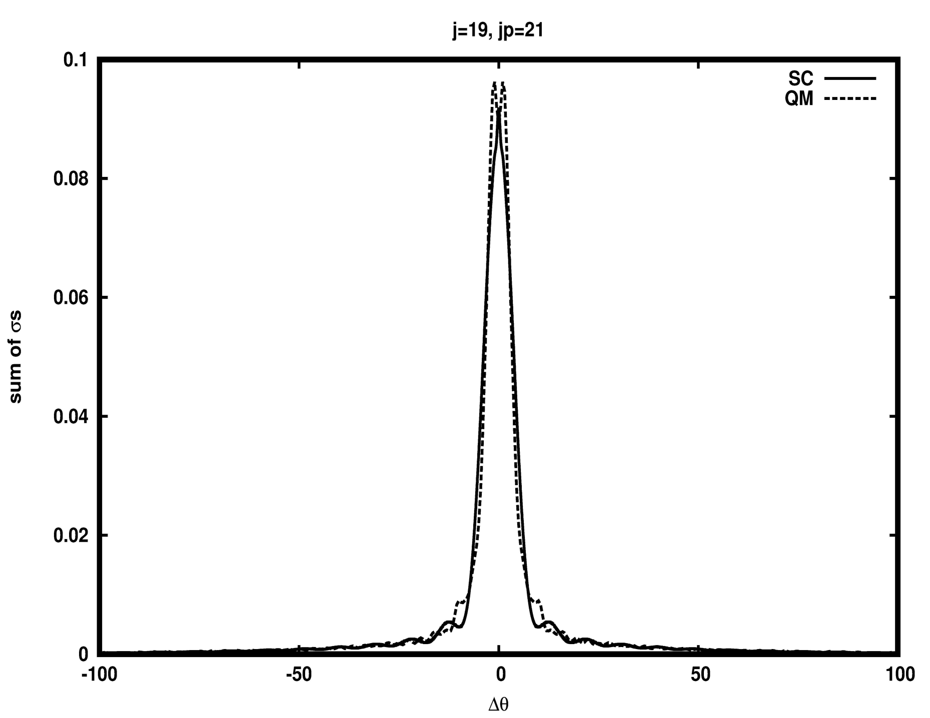


Δj=2

Helium

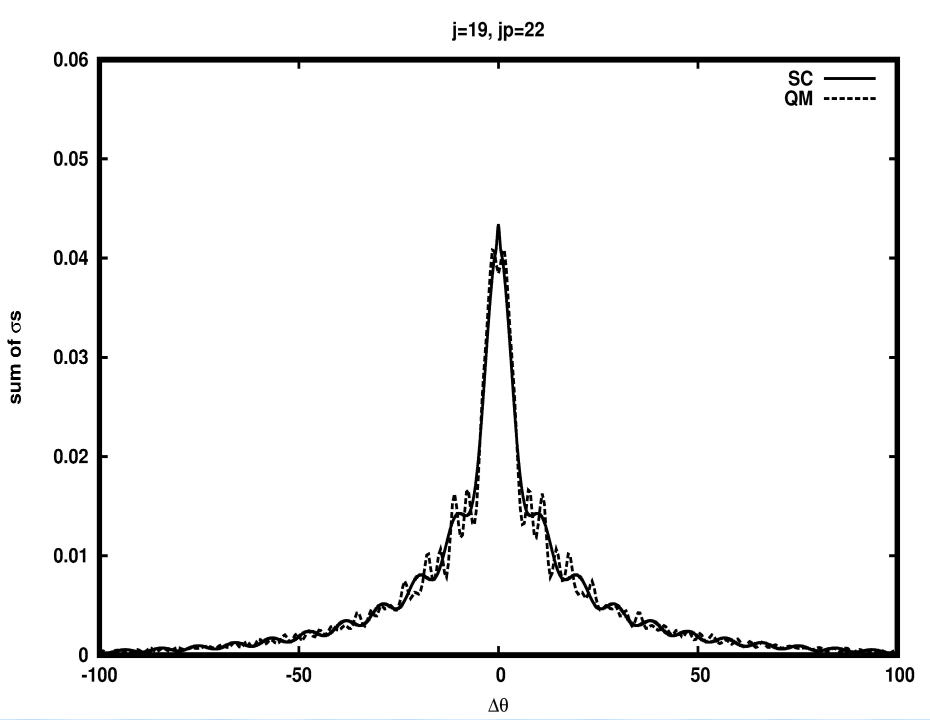
Argon



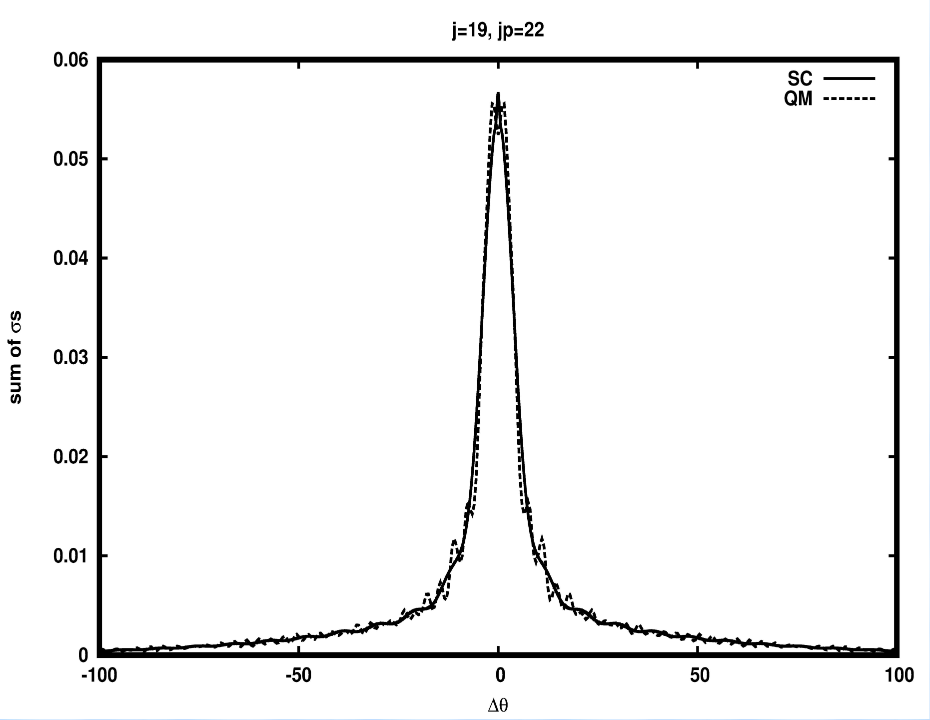


Δj=3

Helium



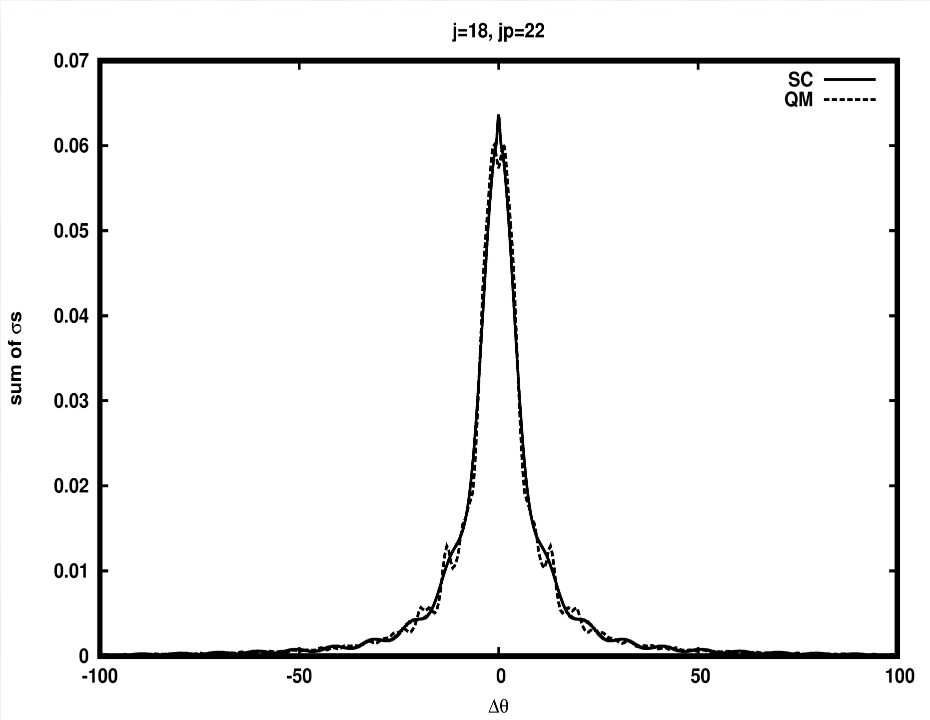
Argon

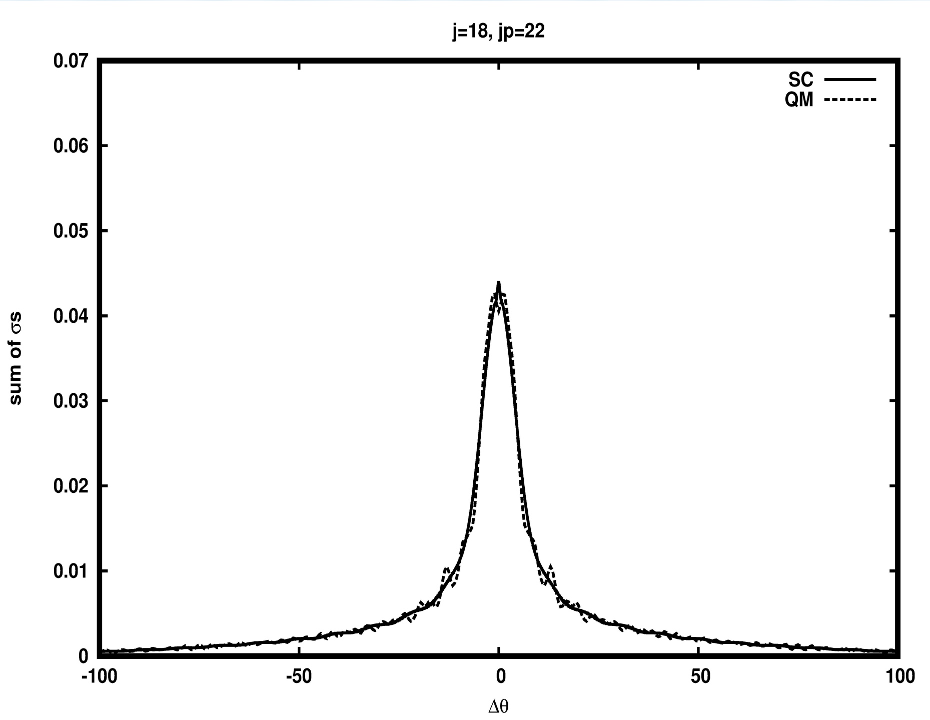


Δj=4

Helium

Argon





Trends in σ

- $\Delta\theta$ tends to be conserved
- As Δj increases, $\Delta\theta$ is less conserved for both
- As Δj increases, Argon σ's distribution becomes more spread out than Helium
- As $\bar{j}$ increases, QM and SC agreement improves, and σ's are less spread out