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S-matrix Method for Extrapolation of the Results of No-Core Shell Model Calculations

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- There are extrapolation methods based on the phenomenological properties of the calculations results
- We suggest a new extrapolation method based on HORSE (it uses an analytical properties of the S-matrix)

HORSE formalism

$$\sum_{N'} (H^L_{NN'} - \delta_{NN'} E) a_{N'L}(k) = 0 \qquad H^L_{NN'} = T^L_{NN'} + V^L_{NN'}$$

$T^L_{N,N+2} = T^L_{N+2,N}$ and T^L_{NN} –kinetic energy non-zero matrix elements

$$N = 2n + L$$

$V^L_{NN'} = 0$ if $N, N' > N_{full}$

$$T^L_{N,N-2} a^{asymp}_{N-2,L}(E) + (T^L_{N,N} - E) a^{asymp}_{N,L}(E) + T^L_{N,N+2} a^{asymp}_{N+2,L}(E) = 0$$

$$a^{asymp}_{NL}(E) = \cos\delta_L S_{NL}(E) + \sin\delta_L C_{NL}(E)$$

$$C^{(\pm)}_{NL}(E) = C_{NL}(E) \pm S_{NL}(E)$$

HORSE formalism

$$S(E)=\frac{C^{(-)}_{N,L}(E)-G_{NN}T^{L}_{N,N+1}C^{(-)}_{N+1,L}(E)}{C^{(+)}_{N,L}(E)-G_{NN}T^{L}_{N,N+1}C^{(+)}_{N+1,L}(E)}$$

$$G_{NN}=-\sum_{\lambda=0}^{N}\frac{\gamma_\lambda^2}{E_\lambda-E}$$

in case of $E=E_\lambda$ $\quad S(E_\lambda)=\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)}$

$$S(E_\lambda)=e^{-2\varphi(\kappa_\lambda)}\left(\frac{\kappa_b+\kappa_\lambda}{\kappa_b-\kappa_\lambda}\right)\left(\frac{\kappa_f+\kappa_\lambda}{\kappa_f-\kappa_\lambda}\right)\left(\frac{\kappa_v-\kappa_\lambda}{\kappa_v+\kappa_\lambda}\right)\left(\frac{(\kappa_\lambda-\gamma)^2+k^2}{(\kappa_\lambda+\gamma)^2+k^2}\right)$$

$$S_L(k_0^*)=\frac{1}{S_0^*},S_L(-k_0^*)=S_0^*,S_L(-k_0)=\frac{1}{S_0}$$

$$E_\lambda=E_\lambda(N_{\max},\hbar\Omega)$$

HORSE formalism

$$\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)} = e^{-2\varphi(\kappa_\lambda)}\left(\frac{\kappa_b+\kappa_\lambda}{\kappa_b-\kappa_\lambda}\right)\left(\frac{\kappa_f+\kappa_\lambda}{\kappa_f-\kappa_\lambda}\right)\left(\frac{\kappa_v-\kappa_\lambda}{\kappa_v+\kappa_\lambda}\right)\left(\frac{(\kappa_\lambda-\gamma)^2+k^2}{(\kappa_\lambda+\gamma)^2+k^2}\right)$$

$$\kappa \sim \sqrt{E}$$

$$E_\lambda = E_\lambda(N_{\max},\hbar\Omega)$$

Extrapolation formulae

$$\frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)$$

1+1 param.

$$\frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)\left(\frac{\sqrt{E_f}+\sqrt{|E_\lambda|}}{\sqrt{E_f}-\sqrt{|E_\lambda|}}\right)$$

1+2 param.

$$\frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}+F\left(\sqrt{|E_\lambda|}\right)^3}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)$$

2+1 param.

$$\Xi = \sqrt{\sum_i \frac{(E_i - E_i^{th})^2}{n}}$$

S-matrix formalism

$$S(E_\lambda) = \frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)}$$

$$S(E_\lambda) = \frac{C_l}{k_\lambda - i\kappa_b}$$ –near to the pole

$$S(E_\lambda) = \frac{1}{\sqrt{2}}\left(\frac{D_l^1}{\sqrt{|E_\lambda|} - \sqrt{|E_\infty^1|}} + \frac{D_l^2}{\sqrt{|E_\lambda|} - \sqrt{|E_\infty^2|}} + \dots\right)$$

$$S(E_\lambda) = \frac{1}{\sqrt{2}}\left(\frac{D_l}{\sqrt{|E_\lambda|} - \sqrt{|E_\infty|}}\right) + B$$

Extrapolation formulae

$$\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)} = \frac{1}{\sqrt{2}}\left(\frac{D_l}{\sqrt{|E_\lambda|} - \sqrt{|E_\infty|}}\right) + B$$

S. A. Coon, Proceedings of the International Workshop on Nuclear Theory in the Supercomputing Era NTSE-2012, Khabarovsk, Russia, June 18–22, 2012. A. M. Shirokov and A. I. Mazur, Editors. Pacific National University, Khabarovsk, Russia, 2013, pp. 171–189.
S. A. Coon *et al.* Phys. Rev. C. **86**, 054002 (2012)

$$E_\lambda = E_\infty + Ae^{-b/\sqrt{s}}, \quad s = \frac{\hbar\Omega}{N_{\max} + L + \frac{7}{2}}$$

– scaling parameter

$$\Lambda = \sqrt{\hbar\Omega(N_{\max} + L + 3/2)mc^2}$$

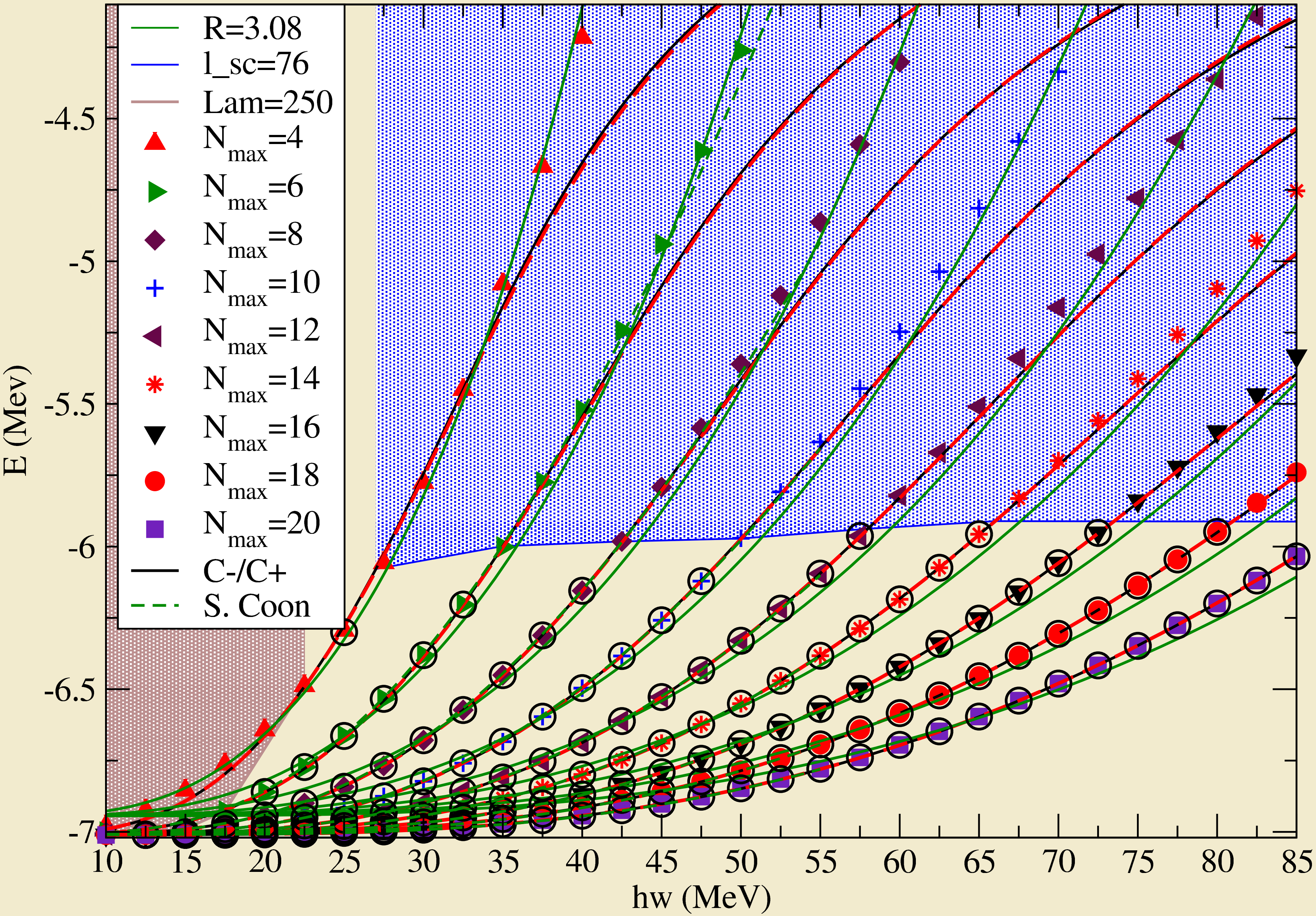
Model problem

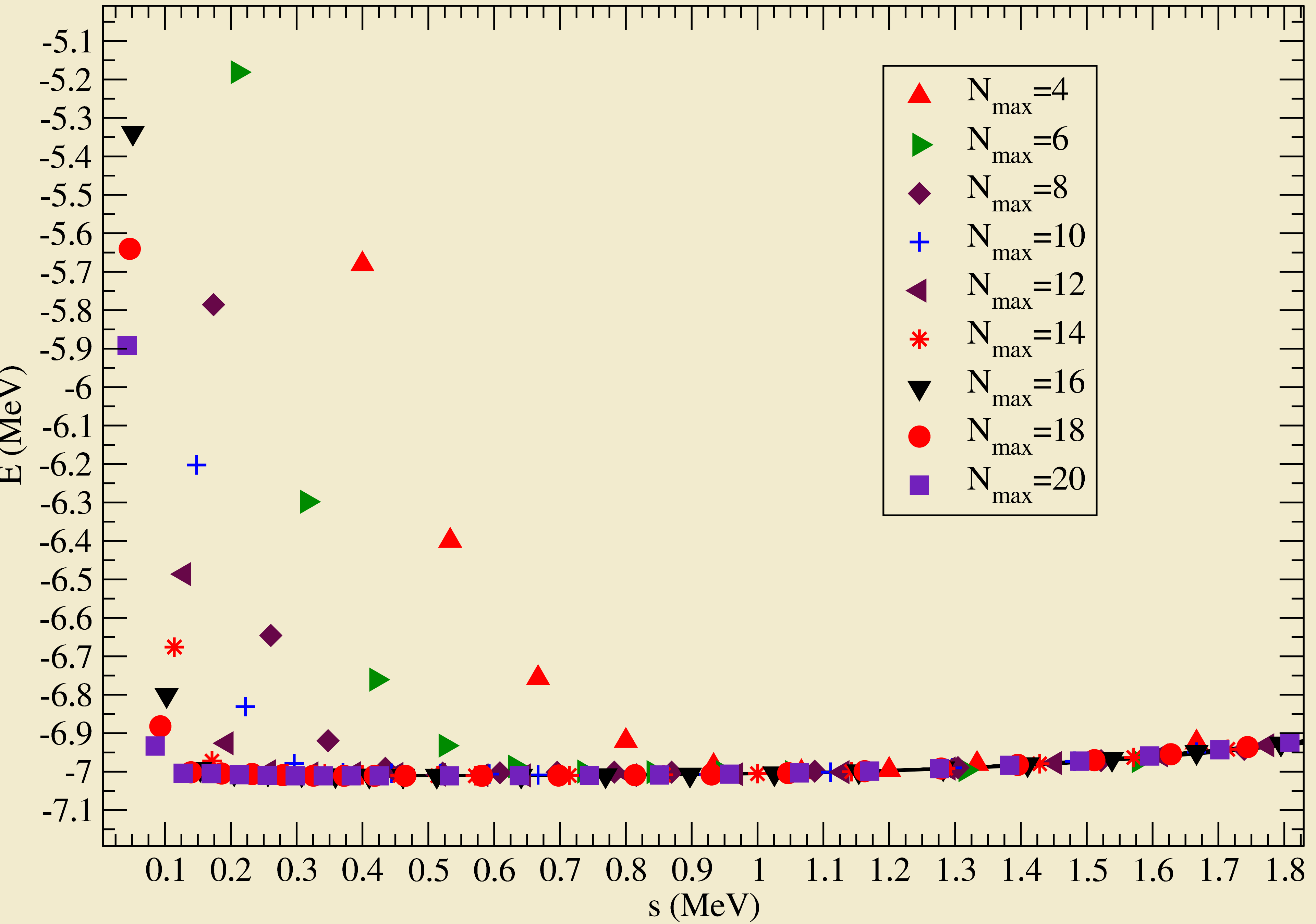
- We are testing the method in case of Woods-Saxon potential:

$$V = \frac{V_0}{1 + \exp[(r - R_0)/a_0]} + (\mathbf{l} \bullet \mathbf{s}) \frac{1}{r} \frac{d}{dr} \frac{V_{ls}}{1 + \exp[(r - R_1)/a_1]}$$

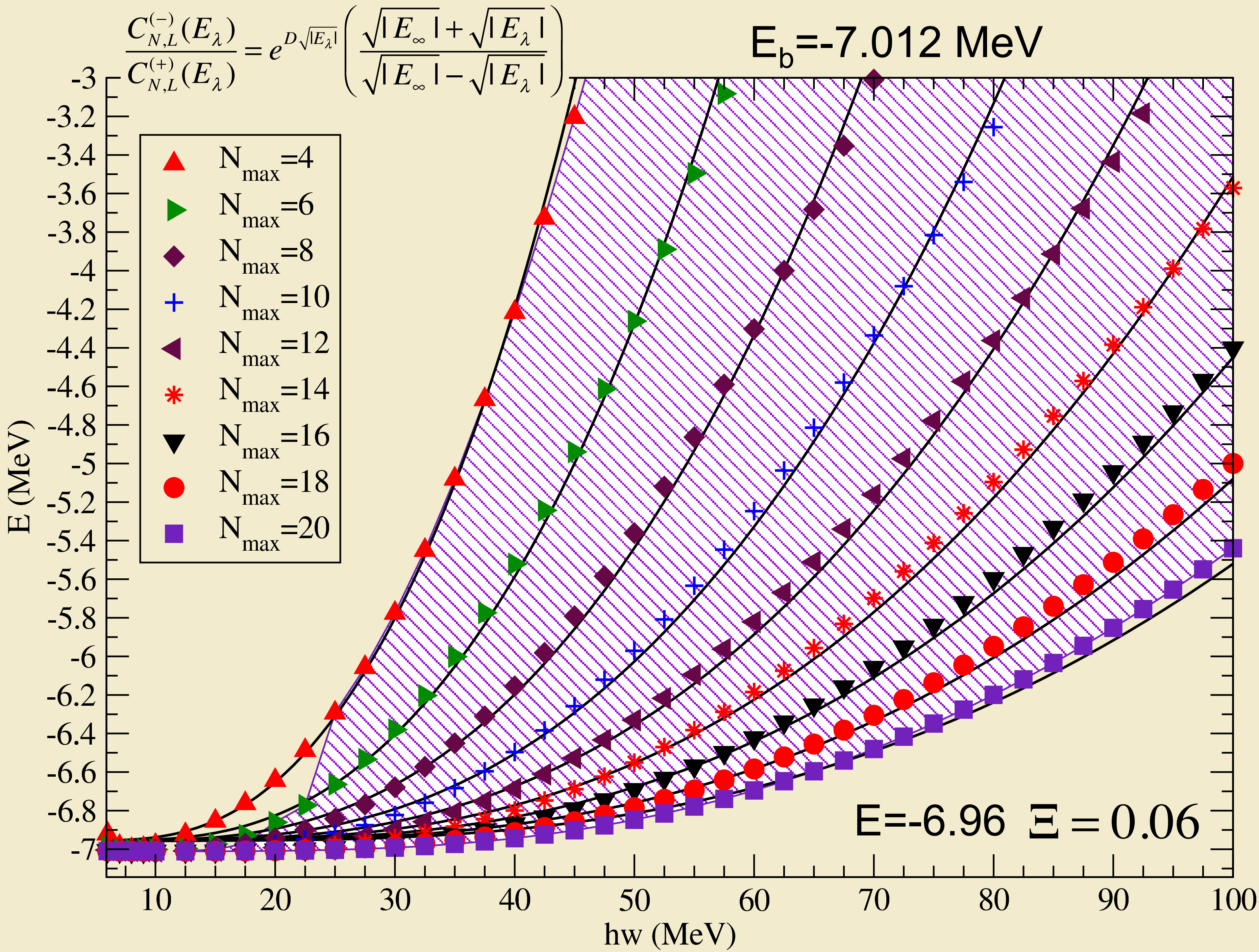
Points selection

$\Lambda_0 = 250 MeV/c$



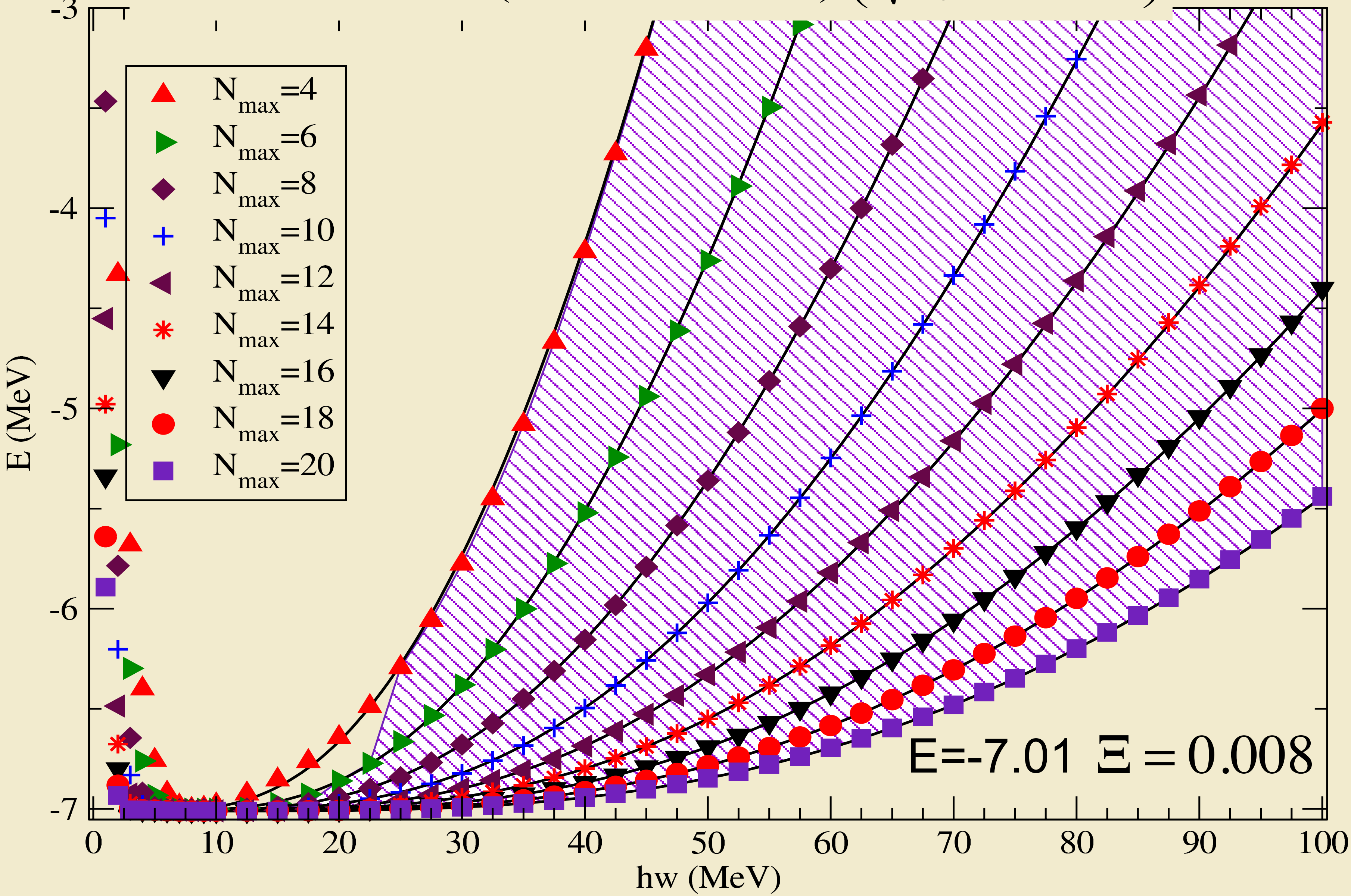


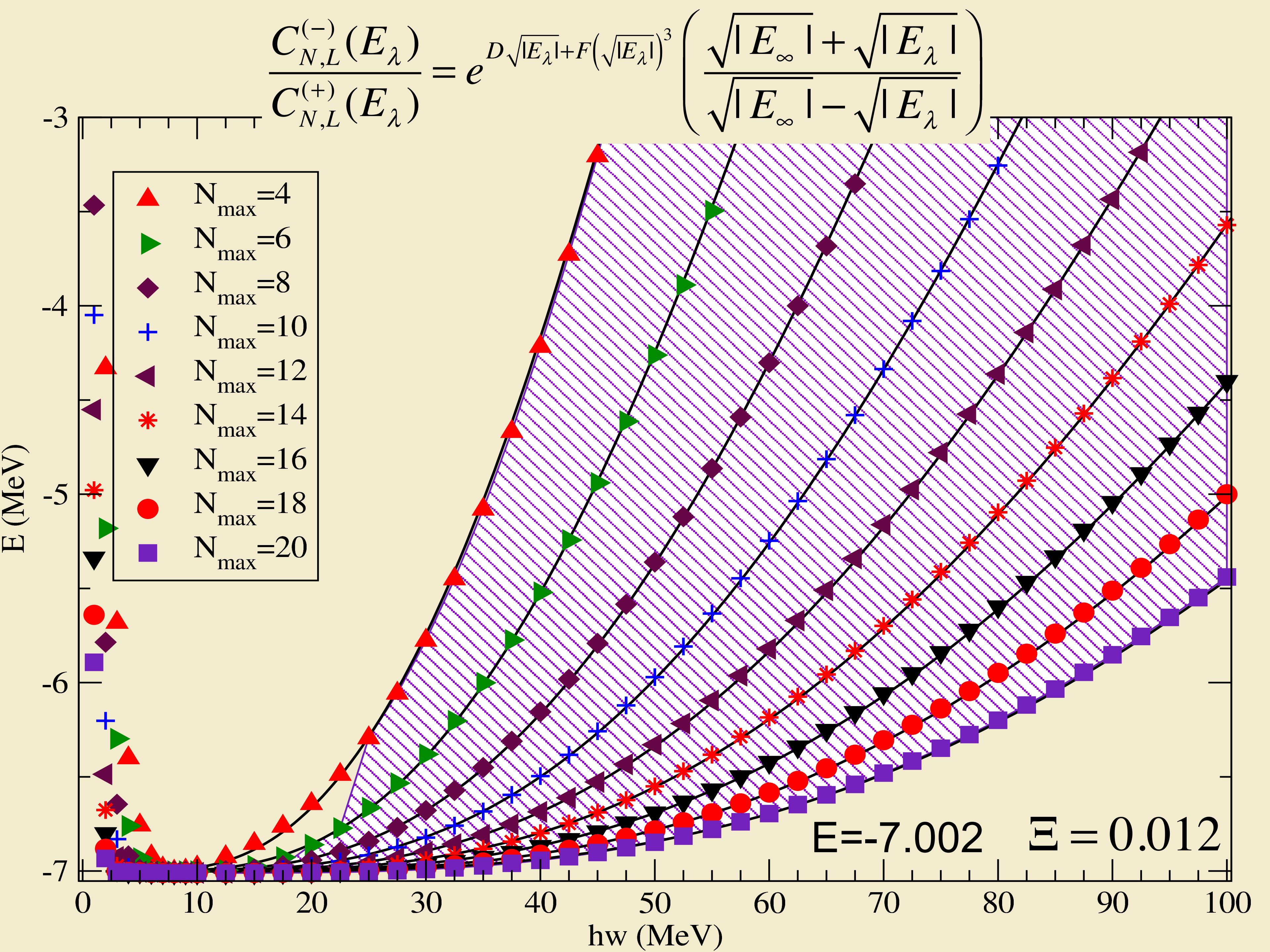
E (MeV)
-5.1
-5.2
-5.3
-5.4
-5.5
-5.6
-5.7
-5.8
-5.9
-6
-6.1
-6.2
-6.3
-6.4
-6.5
-6.6
-6.7
-6.8
-6.9
-7
-7.1
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
s (MeV)
$N_{max}=4$
$N_{max}=6$
$N_{max}=8$
$N_{max}=10$
$N_{max}=12$
$N_{max}=14$
$N_{max}=16$
$N_{max}=18$
$N_{max}=20$



$$\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)$$
E_b=-7.012 MeV
N_{max}=4
N_{max}=6
N_{max}=8
N_{max}=10
N_{max}=12
N_{max}=14
N_{max}=16
N_{max}=18
N_{max}=20
E=-6.96 $\Xi = 0.06$
E (MeV)
hw (MeV)

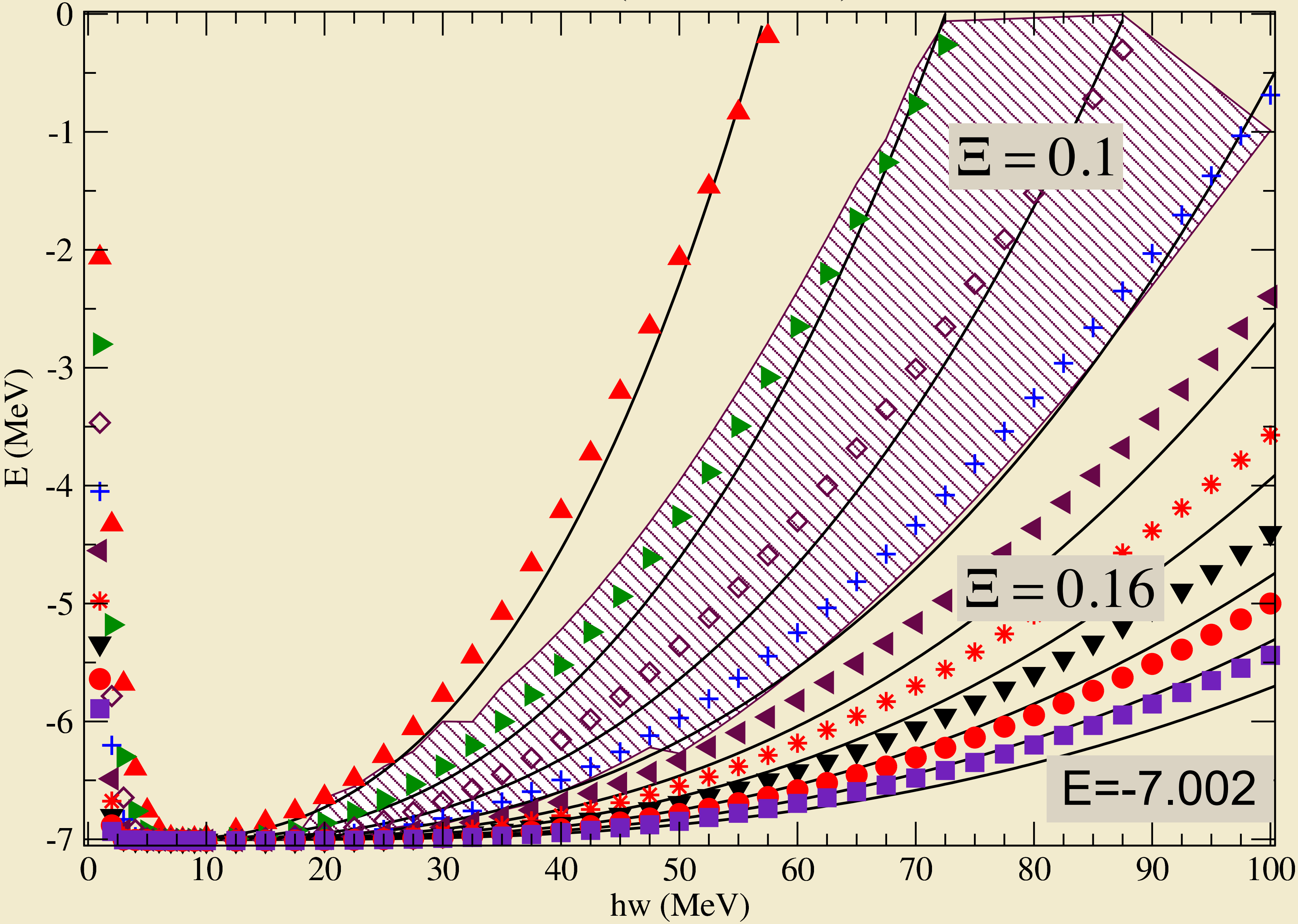
$$\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}} \left(\frac{\sqrt{|E_\infty|} + \sqrt{|E_\lambda|}}{\sqrt{|E_\infty|} - \sqrt{|E_\lambda|}} \right) \left(\frac{\sqrt{E_f} + \sqrt{|E_\lambda|}}{\sqrt{E_f} - \sqrt{|E_\lambda|}} \right)$$



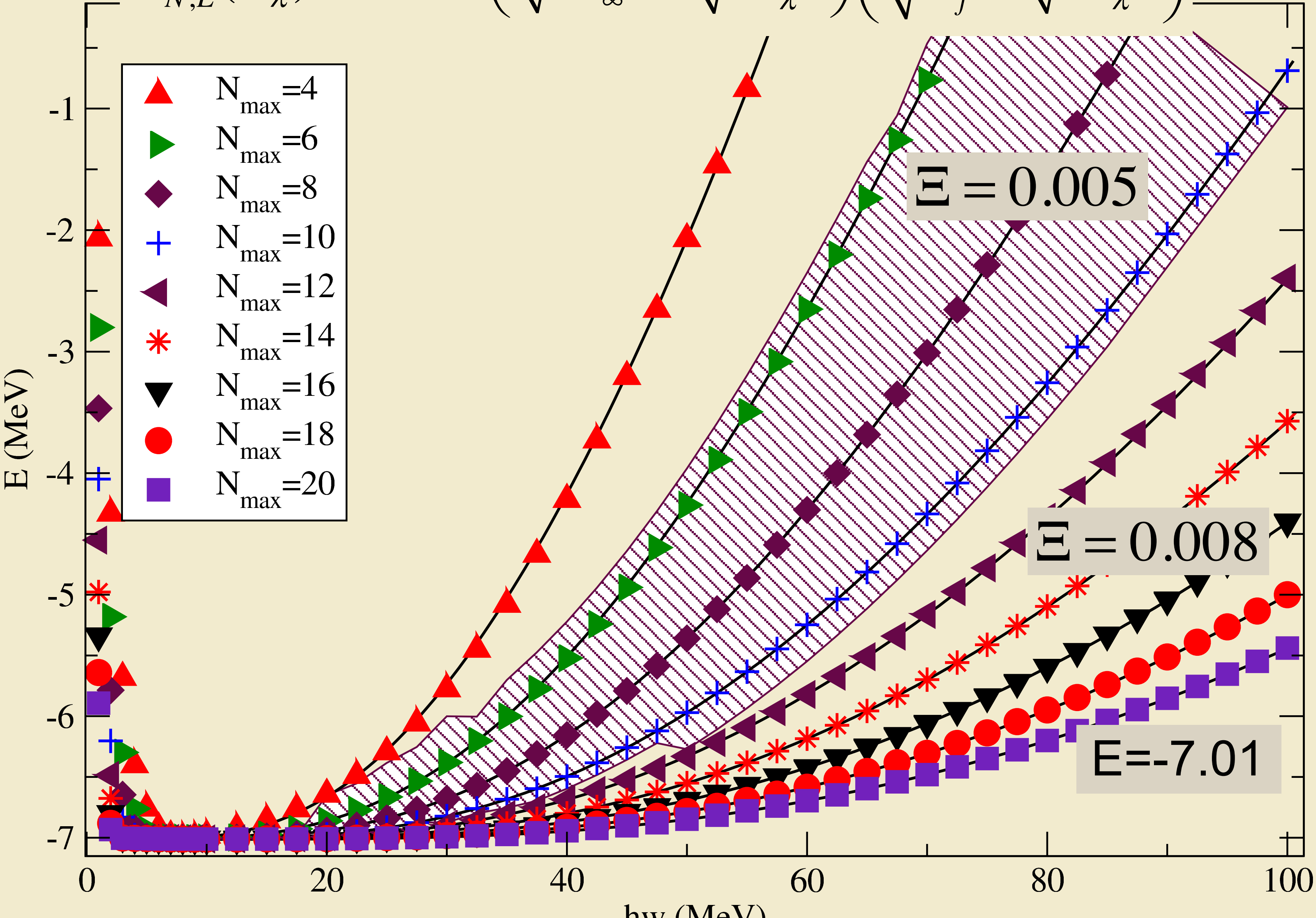


$$\frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}+F\left(\sqrt{|E_\lambda|}\right)^3}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)$$
$N_{max}=4$
$N_{max}=6$
$N_{max}=8$
$N_{max}=10$
$N_{max}=12$
$N_{max}=14$
$N_{max}=16$
$N_{max}=18$
$N_{max}=20$
E=-7.002 $\Xi = 0.012$
E (MeV)
hw (MeV)
-3
-4
-5
-6
-7
0
10
20
30
40
50
60
70
80
90
100

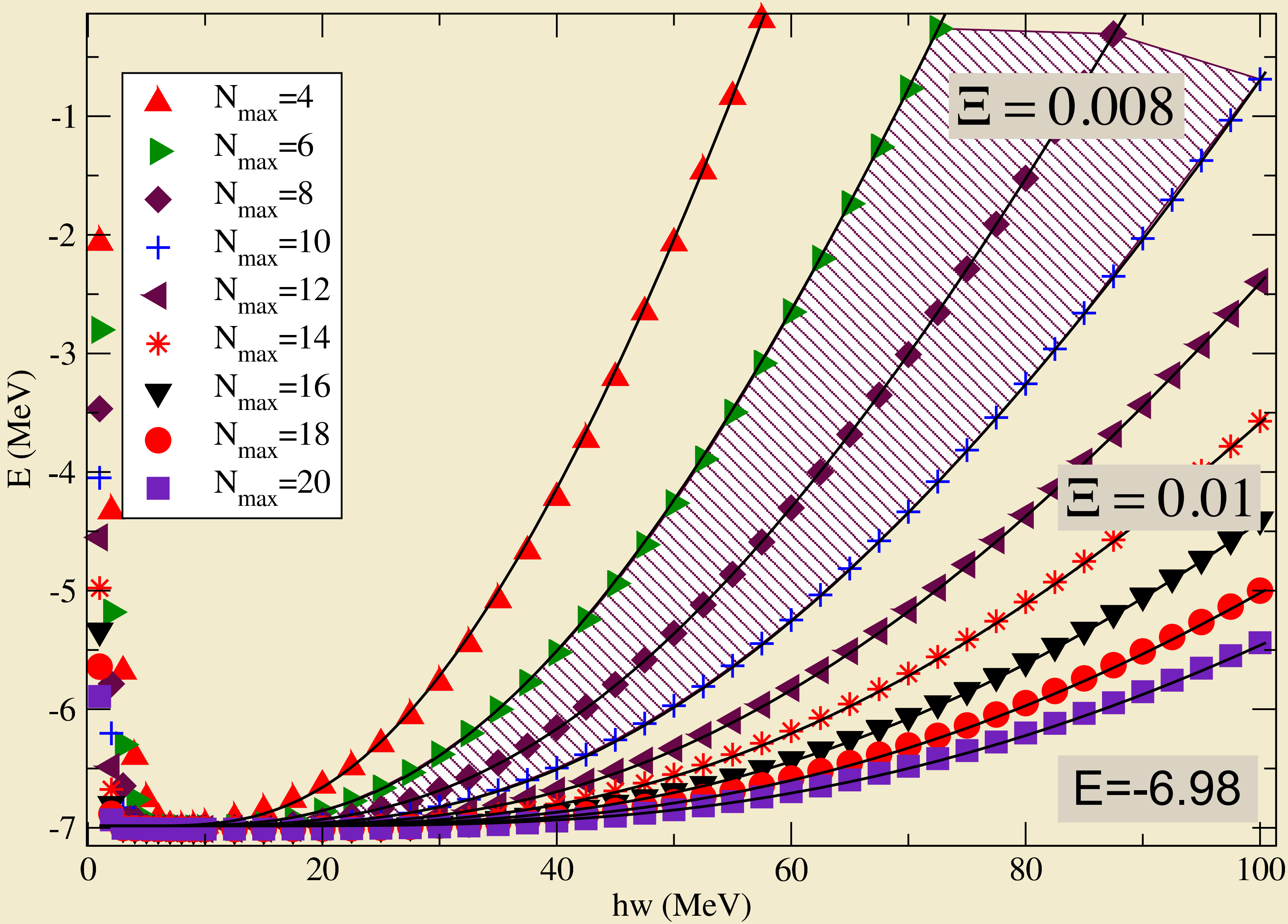
$$\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)$$



$$\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}} \left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)\left(\frac{\sqrt{E_f}+\sqrt{|E_\lambda|}}{\sqrt{E_f}-\sqrt{|E_\lambda|}}\right)$$



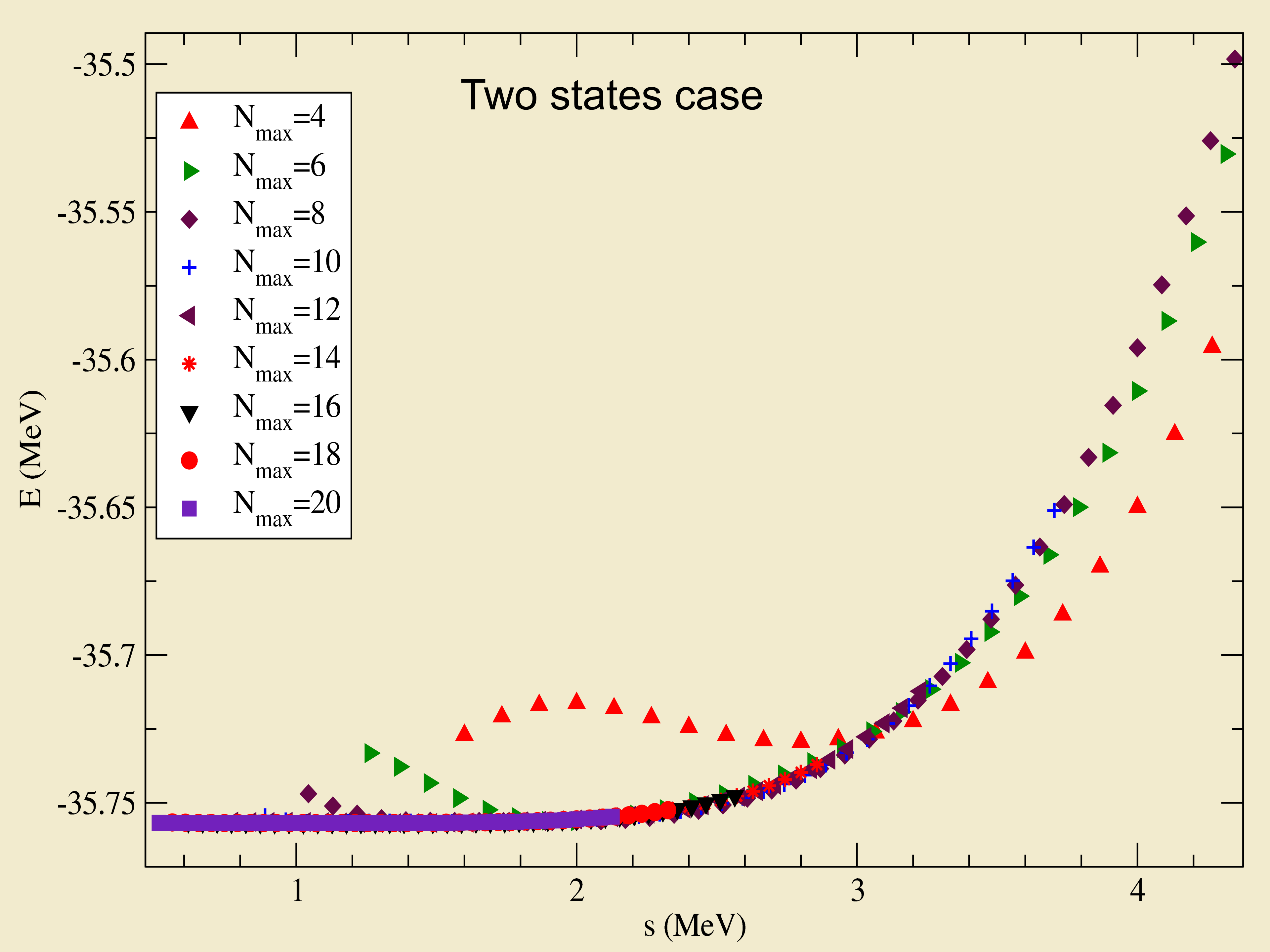
$$E_\lambda = E_\infty + Ae^{-b/\sqrt{s}}$$



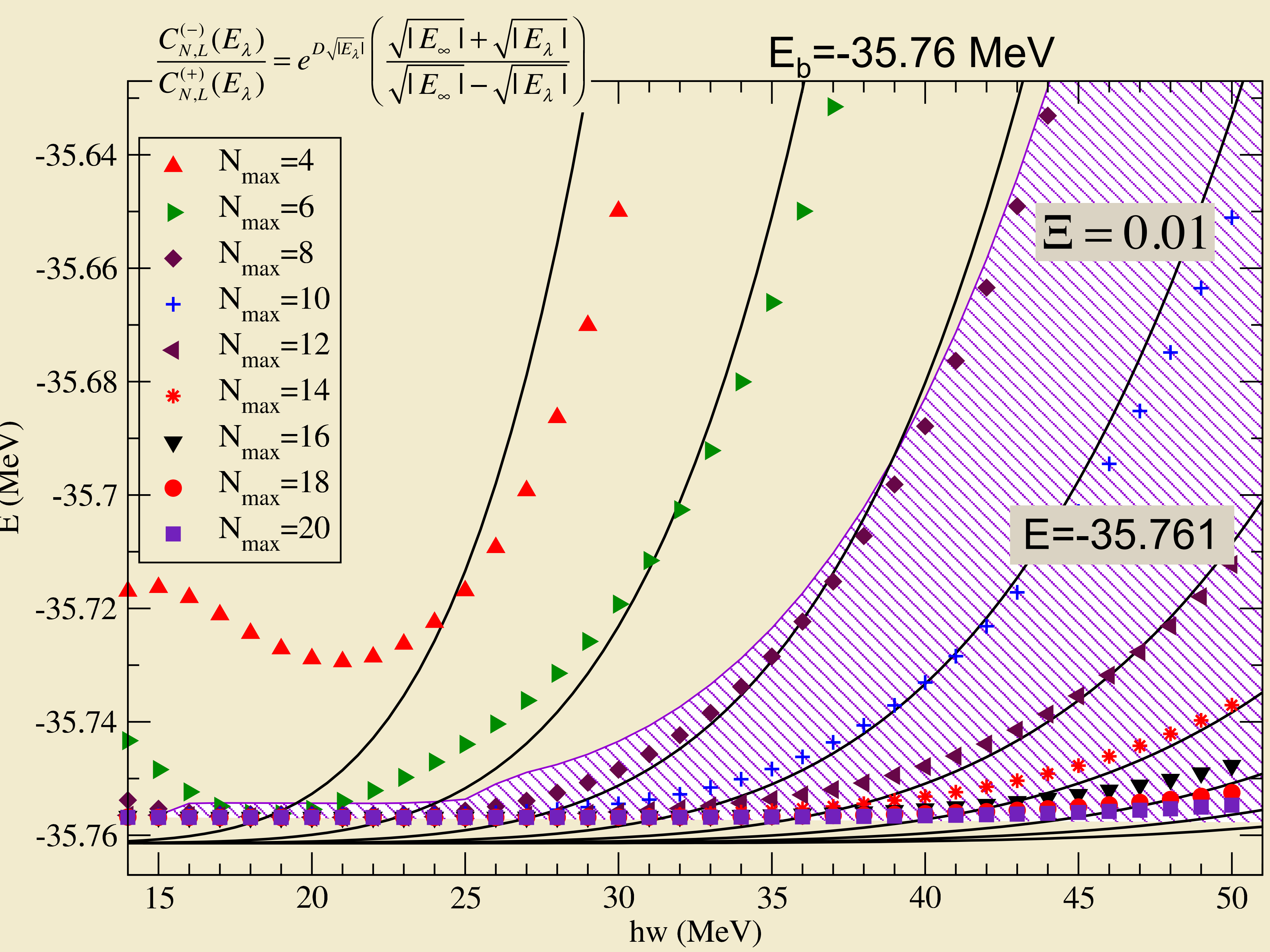
	E_∞ (MeV)	rms (MeV)	D $(MeV)^{-1/2}$	F $(MeV)^{-3/2}$	E_f (MeV)
Energy	-7.012				
1+1 param	-6.96	0.06	0.73		
1+2 param	-7.010	0.008	0.18		15.7
2+1 param	-7.002	0.012	0.68	0.01	
3 param (S.Coon)	-7.025	0.11			

N_{max} 6-10 prediction

	E_∞ (MeV)	rms 6-10	rms full	D $(MeV)^{-1/2}$	F $(MeV)^{-3/2}$	E_f (MeV)
1+1 param	-7.002	0.1	0.16	0.69		
1+2 param	-7.013	0.005	0.008	0.18		15.6
2+1 param	-6.997	0.009	0.01	0.68	0.01	
3 param (S.Coon)	-6.98	0.008	0.01			

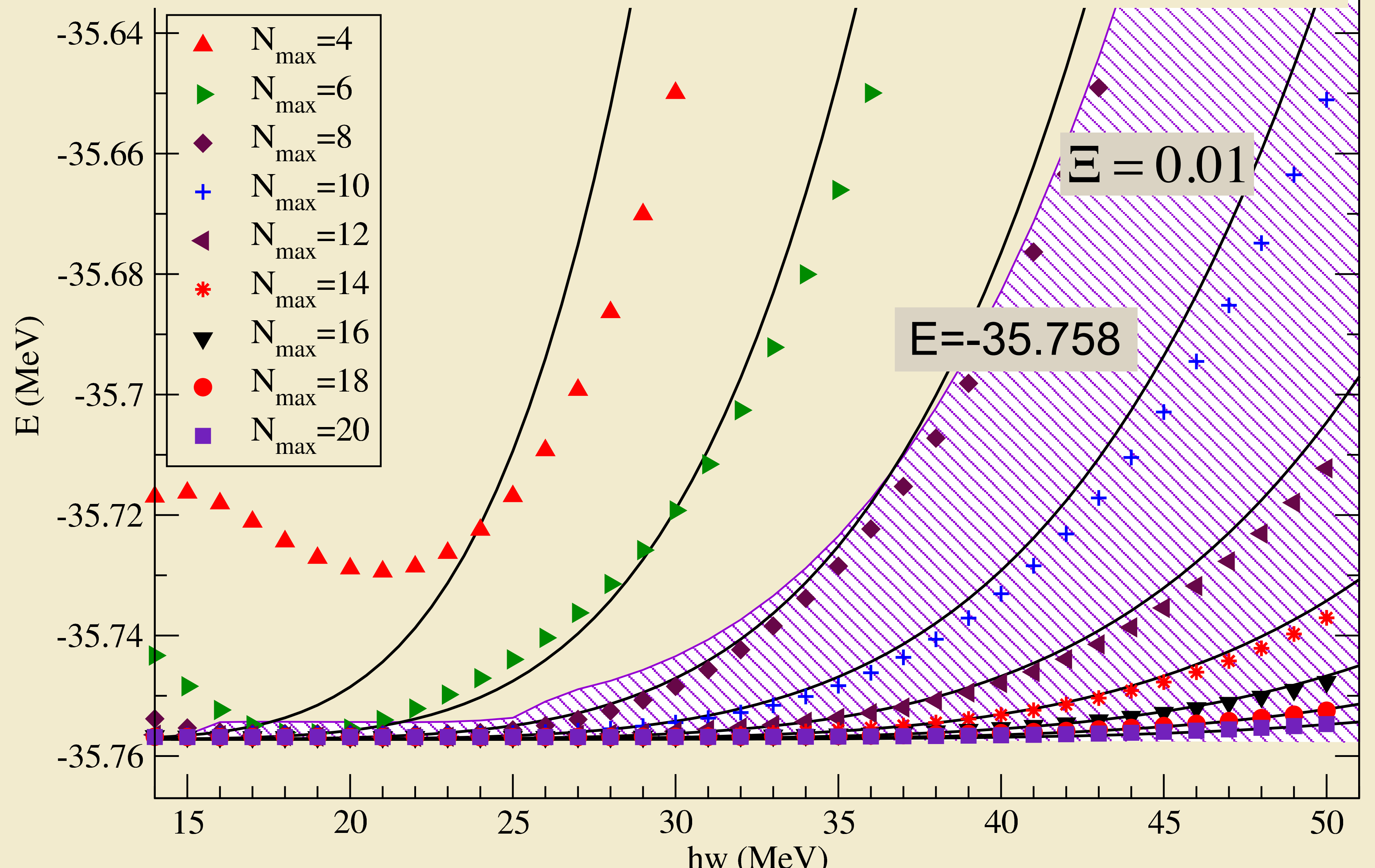


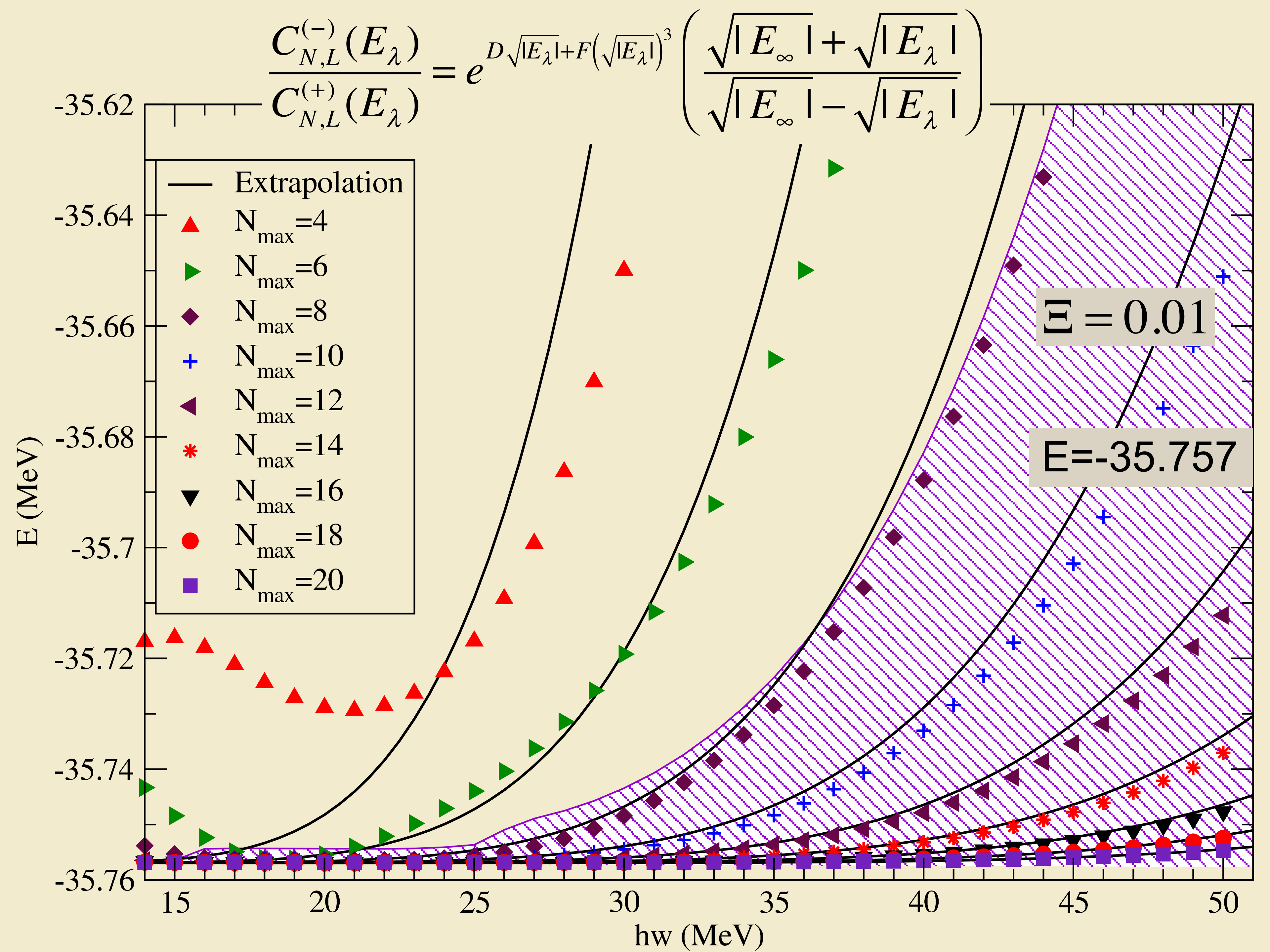
Two states case
N_max=4
N_max=6
N_max=8
N_max=10
N_max=12
N_max=14
N_max=16
N_max=18
N_max=20
E (MeV)
s (MeV)
-35.5
-35.55
-35.6
-35.65
-35.7
-35.75
1
2
3
4



$\frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)$
E_b=-35.76 MeV
$\Xi = 0.01$
E=-35.761
N_{max}=4
N_{max}=6
N_{max}=8
N_{max}=10
N_{max}=12
N_{max}=14
N_{max}=16
N_{max}=18
N_{max}=20
E (MeV)
-35.64
-35.66
-35.68
-35.7
-35.72
-35.74
-35.76
hw (MeV)
15
20
25
30
35
40
45
50

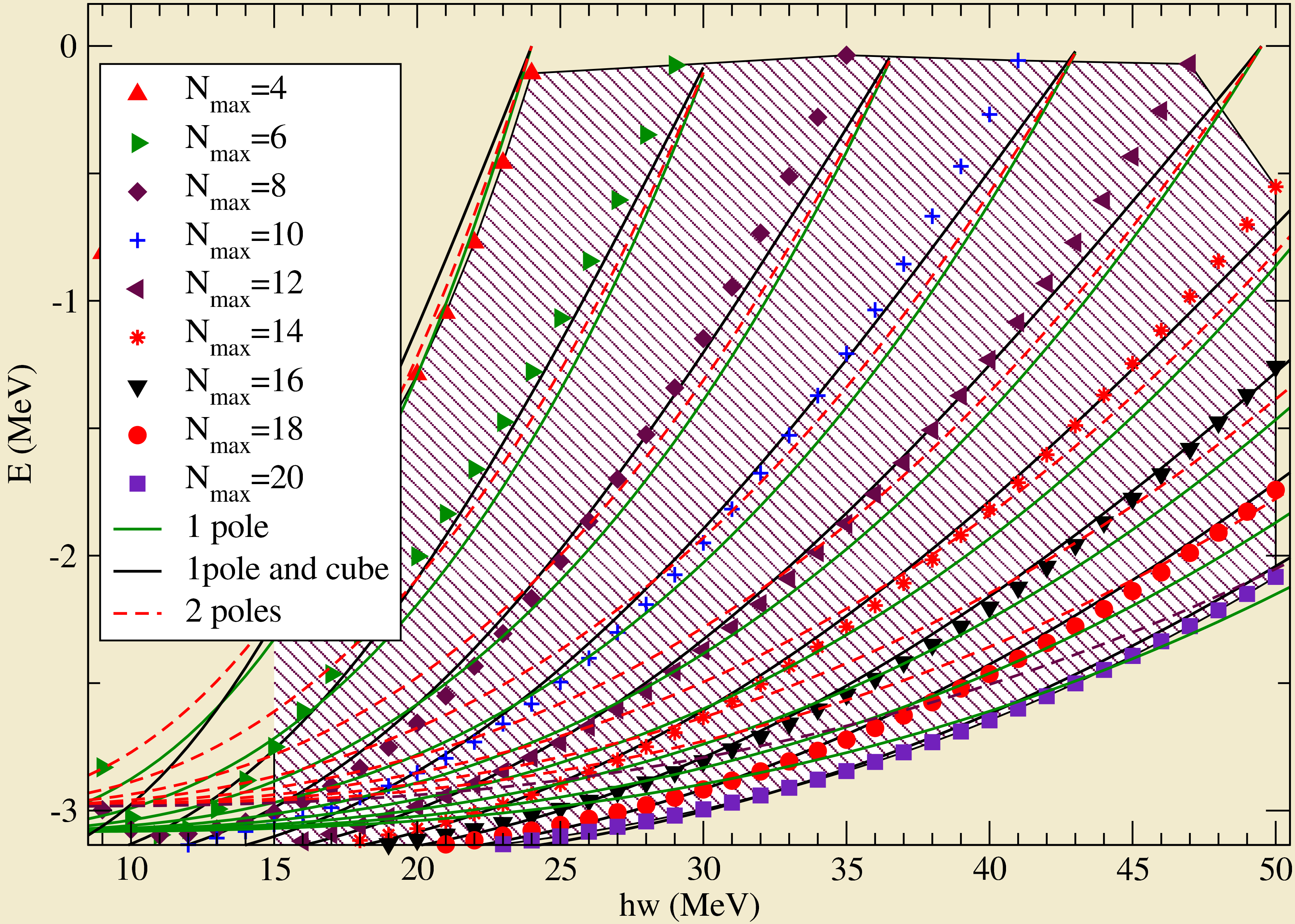
$$\frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}} \left(\frac{\sqrt{|E_\infty|} + \sqrt{|E_\lambda|}}{\sqrt{|E_\infty|} - \sqrt{|E_\lambda|}} \right) \left(\frac{\sqrt{|E_\nu|} - \sqrt{|E_\lambda|}}{\sqrt{|E_\nu|} + \sqrt{|E_\lambda|}} \right) \left(\frac{\sqrt{3.3} + \sqrt{|E_\lambda|}}{\sqrt{3.3} - \sqrt{|E_\lambda|}} \right)$$





$$\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}+F\left(\sqrt{|E_\lambda|}\right)^3}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)$$
Extrapolation
N_{max}=4
N_{max}=6
N_{max}=8
N_{max}=10
N_{max}=12
N_{max}=14
N_{max}=16
N_{max}=18
N_{max}=20
$\Xi = 0.01$
E=-35.757
E (MeV)
hw (MeV)
-35.62
-35.64
-35.66
-35.68
-35.7
-35.72
-35.74
-35.76
15
20
25
30
35
40
45
50

Results for excited state



$$\frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)\left(\frac{\sqrt{|E_v|}-\sqrt{|E_\lambda|}}{\sqrt{|E_v|}+\sqrt{|E_\lambda|}}\right)\left(\frac{\sqrt{36}+\sqrt{|E_\lambda|}}{\sqrt{36}-\sqrt{|E_\lambda|}}\right)$$

1+1 param	-35.761	0.01	0.92		
1+2 param	-35.758	0.01	1.13		20.1
2+1 param	-35.757	0.01	0.62	0.01	

$$\frac{C_{N,L}^{(-)}(E_\lambda)}{C_{N,L}^{(+)}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)\left(\frac{\sqrt{|E_v|}-\sqrt{|E_\lambda|}}{\sqrt{|E_v|}+\sqrt{|E_\lambda|}}\right)\left(\frac{\sqrt{3.3}+\sqrt{|E_\lambda|}}{\sqrt{3.3}-\sqrt{|E_\lambda|}}\right)$$

exc.st.	-3.6				
1+1 param	-3.08	0.14	1.1		
1+2 param	-2.98	0.17	1.92		33
2+1 param	-3.25	0.06	1.1	0.05	
S.Coon	-3.22	0.04			

Conclusions

- We suggest a new method for extrapolations of calculations in oscillator basis.
- It provides adequate binding energies

$$\frac{C^{(-)}_{N,L}(E_\lambda)}{C^{(+)}_{N,L}(E_\lambda)} = e^{D\sqrt{|E_\lambda|}+F\left(\sqrt{|E_\lambda|}\right)^3}\left(\frac{\sqrt{|E_\infty|}+\sqrt{|E_\lambda|}}{\sqrt{|E_\infty|}-\sqrt{|E_\lambda|}}\right)$$

Thank you for attention!