Ab-Initio No Core Shell Model and its Relation to Physics with 12 GeV Electrons

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The Physics of Nuclei with 12 GeV Electrons
TJNL, November 1-5, 2004

I. Ab initio approach to many-fermion/boson systems
II. Results for light nuclei
III. Links to the quark cluster model of nuclei
III. Conclusions and outlook

Constructing a non-perturbative bridge between
"Short distance physics" ⟺ "Long distance physics"

Asymptotically free current quarks Chiral symmetry High momentum transfer processes	⟺	Constituent quarks Broken Chiral symmetry Meson and Baryon Spectroscopy Hadron-Hadron interactions
Bare NN, NNN interactions fitting 2 & 3-body data Short range correlations & strong tensor correlations Bare transition operators	⟺	Effective NN, NNN interactions describing low energy nuclear data Mean field, pairing, & quadrupole, etc., correlations Effective charges, GT quenching, etc.

BOLD CLAIM

We now have the tools to accomplish this program in nuclear many-body theory

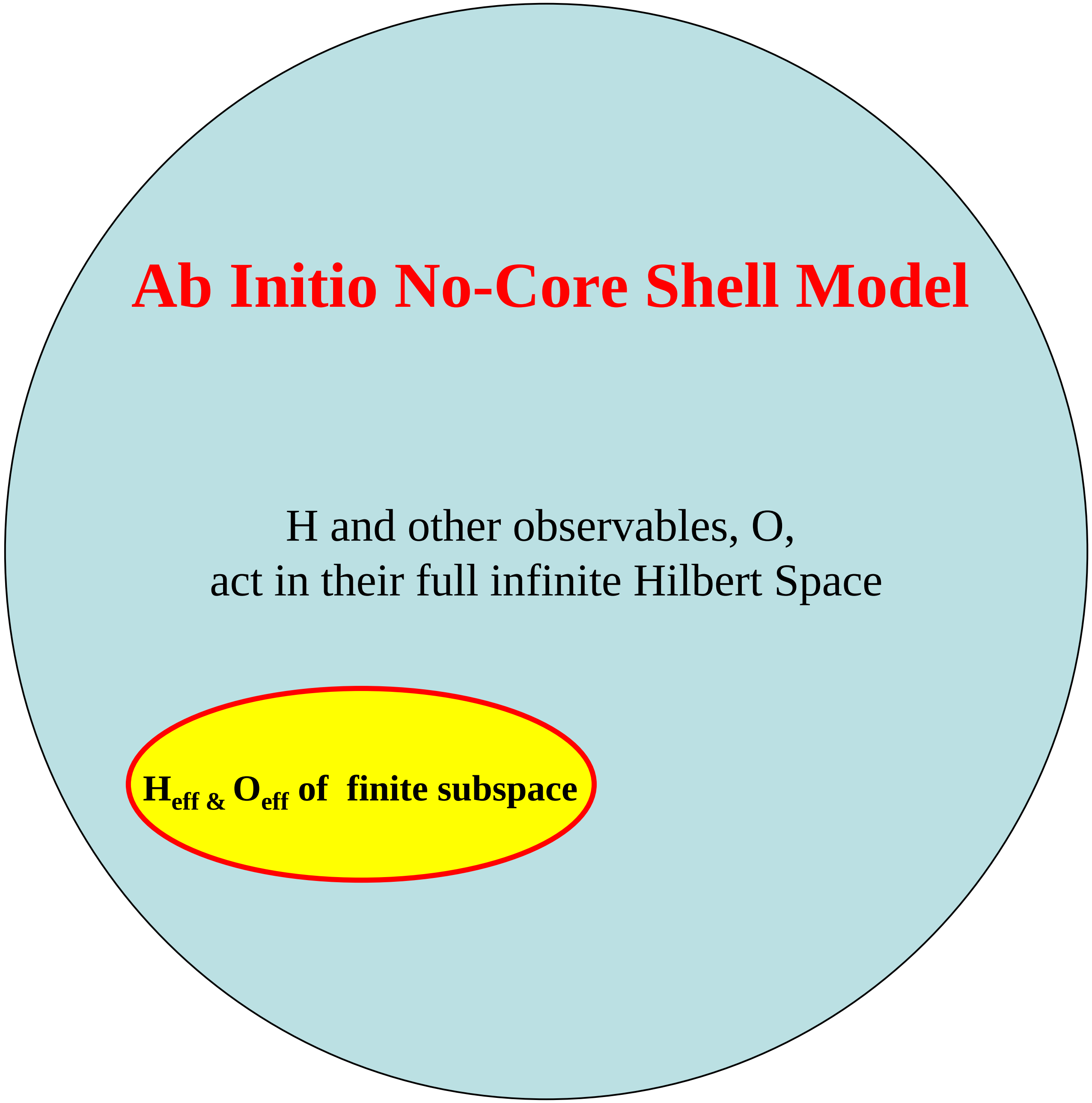
The tools are now sufficiently robust to provide
precision tests of the Hamiltonians themselves
Argonne-LANL-Urbana (GFMC) pioneered this path

New and Emerging NN, NNN interactions fitting NN and NNN data

- Traditional meson-exchange theory (Nijmegen X, CD Bonn X, AVX, etc.,)
- Effective field theory with roots in QCD (EFT X, Idaho X, NXLO, etc.,)
- Renormalization group reduced bare NN interactions (V-lowk X)
- Off-shell variations of bare NN interactions (INOY-X, etc.,)
- Inverse scattering theory (ISTP, JISPX, etc.,)

Hamiltonian fitting NN and NNN data	⇄	Nuclear spectra and other properties

Once these issues resolved, we have the tools to make high precision predictions for tests of fundamental symmetries in nuclear experiments.


Ab Initio No-Core Shell Model
H and other observables, O,
act in their full infinite Hilbert Space
H_{eff} & O_{eff} of finite subspace

Effective Hamiltonian for A-Particles

Lee-Suzuki-Okamoto Method plus Cluster Decomposition

P. Navratil, J.P. Vary and B.R. Barrett,
Phys. Rev. Lett. 84, 5728(2000); Phys. Rev. C62, 054311(2000)
C. Viazminsky and J.P. Vary, J. Math. Phys. 42, 2055 (2001);
K. Suzuki and S.Y. Lee, Progr. Theor. Phys. 64, 2091(1980);
K. Suzuki, *ibid*, 68, 246(1982);
K. Suzuki and R. Okamoto, *ibid*, 70, 439(1983)

Preserves the symmetries of the full Hamiltonian:
Rotational, translational, parity, etc., invariance

$$H_{\mathcal{A}} = T_{rel} + V = \sum_{i<j}^{\mathcal{A}} \left[\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + V_{ij} \right] + V_{NNN}$$

Select a finite oscillator basis space (P-space) and evaluate an a- body cluster effective Hamiltonian:

$$\mathcal{H} = T_{rel} + \mathcal{V}^{(a)}$$

Guaranteed to provide exact answers as $a \rightarrow A$ or as $P \rightarrow 1$.

Introduce similarity transformation acting only on the intrinsic coordinates [Lee-Suzuki-Okamoto]

$$H_{\mathsf{A}} |k\rangle = E_k^{\mathsf{A}} |k\rangle$$

$$\mathcal{H} = e^{-S_{\mathcal{A}}} H_{\mathcal{A}} e^{S_{\mathcal{A}}} = e^{-S_{\mathcal{A}}} \left[H_{\mathcal{A}}^{\Omega} - H_{CM} \right] e^{S_{\mathcal{A}}} = \mathcal{H}^{(1)} + \mathcal{H}^{(\mathcal{A})} - H_{CM}$$

$$\mathcal{H}^{(1)} = H_0 = \sum_i^{\mathcal{A}} h_i = \sum_i^{\mathcal{A}} \left(\frac{p_i^2}{2m} + \frac{1}{2} m \Omega^2 r_i^2 \right)$$

$$|\tilde{k}\rangle = e^{-S_{\mathcal{A}}} |k\rangle$$

$$\mathcal{H} |\tilde{k}\rangle = E_k^{\mathcal{A}} |\tilde{k}\rangle$$

Nothing has happened to the original problem

Define a normalized A - Particle Fock - space basis state:

$$\mathbf{a}^{+}_{\alpha}\mathbf{a}^{+}_{\beta}\cdots\mathbf{a}^{+}_{\zeta}|0\rangle \equiv |\alpha\beta\cdots\zeta\rangle \equiv |\alpha_n\rangle$$

$$H_0|\alpha_n\rangle = \varepsilon_n|\alpha_n\rangle$$

$$\varepsilon_n \equiv \{\varepsilon_\alpha + \varepsilon_\beta + \cdots + \varepsilon_\zeta\}$$

Define the A - particle basis space (P - space) to consist of all basis states { $|\alpha_n\rangle$ **} satisfying:**

$$\varepsilon_n \le \{N_m + 3A/2\}\hbar\Omega$$

$$N_m \equiv N_{\min} + N_{\max}$$

For A - Fermions $N_{\min} \equiv$ **Minimum oscillator quanta [** $\sum$ **(2n + l)] satisfying the Pauli Principle.**

We characterize the P - space by quoting " $\mathbf{N}_{\mathbf{max}}\hbar\Omega$**"**

Notation: $\{|\alpha_n\rangle\}_{\mathbf{P}} \equiv \{|\alpha_P\rangle\}$

Define the finite basis (P-space) effective Hamiltonian

Introduce A-fermion basis space projectors P and Q

$$P_A = \sum_{P \in \mathbf{P}} |\alpha_P\rangle\langle\alpha_P|$$

$$Q_A = \sum_{Q \in \mathbf{Q}} |\alpha_Q\rangle\langle\alpha_Q|$$

$$P_A + Q_A = 1_A$$

$$P_A^2 = P_A \quad Q_A^2 = Q_A \quad P_A Q_A = 0$$

Require the similarity transform to satisfy decoupling condition => separate Hermitian effective Hamiltonians for P&Q spaces

$$[P_{\mathcal{A}} + Q_{\mathcal{A}}]\mathcal{H}[P_{\mathcal{A}} + Q_{\mathcal{A}}]|\tilde{k}\rangle = E_k^{\mathcal{A}}[P_{\mathcal{A}} + Q_{\mathcal{A}}]|\tilde{k}\rangle$$

$$P_{\mathcal{A}}\mathcal{H}Q_{\mathcal{A}} = 0 = Q_{\mathcal{A}}\mathcal{H}P_{\mathcal{A}}$$

$$=> P_{\mathcal{A}}\mathcal{H}P_{\mathcal{A}}|\tilde{k}\rangle = E_k^{\mathcal{A}}P_{\mathcal{A}}|\tilde{k}\rangle, \; k = 1,,,d$$

$$=> Q_{\mathcal{A}}\mathcal{H}Q_{\mathcal{A}}|\tilde{k}\rangle = E_k^{\mathcal{A}}Q_{\mathcal{A}}|\tilde{k}\rangle, \; k = d+1,...\infty$$

Still no approximations to the original problem

Formal solution to the full decoupling problem

Instructive for the cluster approximation

$$H_{\mathcal{A}}|k\rangle = E_k^{\mathcal{A}}|k\rangle$$

$$|\tilde{k}\rangle = e^{-S_{\mathcal{A}}}|k\rangle$$

$$\mathcal{H} = e^{-S_{\mathcal{A}}} H e^{S_{\mathcal{A}}}$$

$$S_{\mathcal{A}} = \operatorname{arctan} h(\omega - \omega^T)$$

$$\omega = Q_{\mathcal{A}} \omega P_{\mathcal{A}}$$

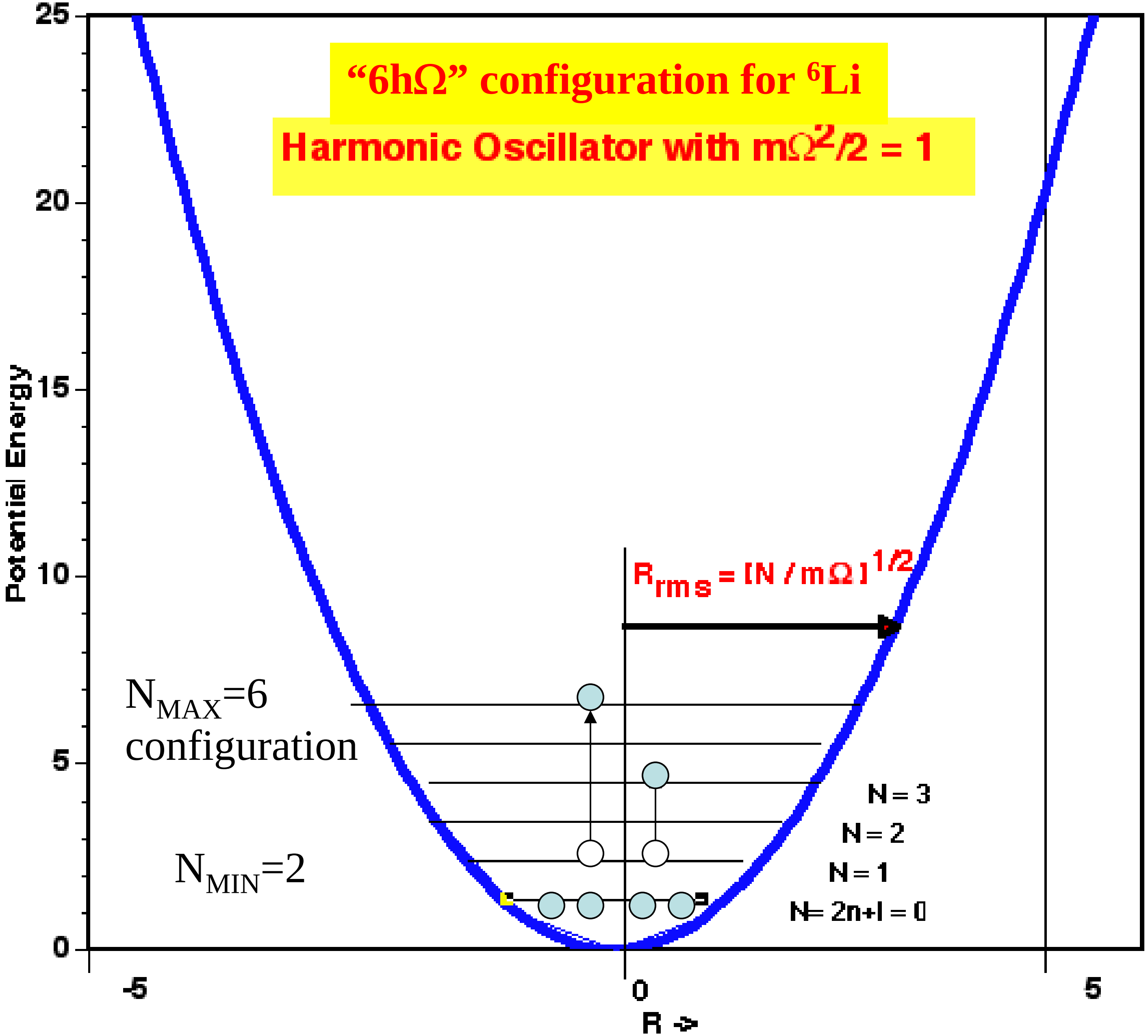
$$\langle \alpha_Q | \omega | \alpha_P \rangle = \sum_{k \in K} \langle \alpha_Q | k \rangle \langle \hat{k} | \alpha_P \rangle$$

$$where: \langle \hat{k} | \alpha_P \rangle = Inverse\{\langle k | \alpha_P \rangle\}$$

Provides formal solution in a convenient form

$$\mathcal{H} = (P_{\mathcal{A}} + \omega^T \omega)^{-1/2} (P_{\mathcal{A}} + P_{\mathcal{A}} \omega^T Q_{\mathcal{A}}) H_{\mathcal{A}} (Q_{\mathcal{A}} \omega P_{\mathcal{A}} + P_{\mathcal{A}}) (P_{\mathcal{A}} + \omega^T \omega)^{-1/2}$$

The same transformation applies to other observables.
Still nothing has happened to the original problem except
a similarity transformation which ***preserves all observables***



"6hΩ" configuration for 6Li
Harmonic Oscillator with mΩ2/2 = 1
Rrms = [N / mΩ]1/2
NMAX=6
configuration
NMIN=2
N = 3
N = 2
N = 1
N= 2n+l = 0
Potential Energy
R ->
25
20
15
10
5
0
-5
0
5

Motivation for this definition of P-space

1. All states up to cutoff (N_m) in unperturbed quanta are retained. Thus, the more realistic our choice of H_o, the more rapidly we expect convergence with cutoff.

2. We can <u>exactly</u> retain translational invariance in this overcomplete basis (3A degrees of freedom vs. 3A-3 intrinsic) using a Lagrange multiplier (Lipkin-Lawson projection method):

$$H \rightarrow H + \lambda(H_{CM} - \frac{3}{2}\hbar\Omega)$$

With H acting only on intrinsic coordinates and λ chosen sufficiently large, we obtain a spectroscopy:

$$\left.\begin{array}{l} \equiv\equiv\equiv\equiv\equiv\equiv\equiv\equiv\ N_{cm} = 2 \\ \updownarrow \lambda\hbar\Omega \\ \equiv\equiv\equiv\equiv\equiv\equiv\equiv\equiv\ N_{cm} = 1 \end{array}\right\} \text{States with spurious CM motion}$$

$$\updownarrow \lambda\hbar\Omega$$

$$\left.\equiv\equiv\equiv\equiv\equiv\equiv\equiv\equiv\ N_{cm} = 0 \right\} \text{Physically relevant states}$$

Cluster Approximation

*Assume the model-space **A**-body effective Hamiltonian is a superposition of **a**-body cluster effective Hamiltonians*

$$\mathcal{H} \approx \mathcal{H}^{(1)} + \mathcal{H}^{(a)} - H_{CM}$$

$$= \mathcal{H}^{(1)} + \frac{\binom{\mathcal{A}}{2}}{\binom{\mathcal{A}}{a}\binom{a}{2}} \sum_{i_1 < i_2 < i_3 < \ldots i_a}^{\mathcal{A}} \tilde{V}_{i_1 i_2 i_3 \ldots i_a} - H_{CM}$$

$$\tilde{V}_{123\ldots a} = e^{-S_a} H^{\Omega}_{a,A} e^{S_a} - \sum_i^a h_i$$

Key equations to solve at the a-body cluster level

Solve a cluster eigenvalue problem in a very large but finite harmonic oscillator basis and retain all the symmetries of the bare Hamiltonian

$$P_a = \sum_{P \in \mathbf{P}} |\alpha_P\rangle\langle\alpha_P|$$

$$Q_a = \sum_{Q \in \mathbf{Q}} |\alpha_Q\rangle\langle\alpha_Q|$$

$$P_a + Q_a \approx 1_a$$

$$H^{\Omega}_{a,A} |k\rangle = E_k |k\rangle$$

$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k \in K} \langle\alpha_Q|k\rangle\langle\hat{k}|\alpha_P\rangle$$

$$where : \langle\hat{k}|\alpha_P\rangle = Inverse\ \{\langle k|\alpha_P\rangle\}$$

$$\mathcal{H}^{(a)} = (P_a + \omega^T\omega)^{-1/2}(P_a + P_a\omega^T Q_a)H^{\Omega}_{a,A}(Q_a\omega P_a + P_a)(P_a + \omega^T\omega)^{-1/2}$$

Ab-initio no-core shell model (NCSM) results

a = 2 for 2 < A < 16, 47, 48, 49

a = 3 for 3 < A < 16

Results in a harmonic oscillator basis space

P_A characterized by:

$$N_m = \sum_{i \in \alpha_P} (2n_i + l_i) \le N_{\min} + \boxed{N_{\max}}$$

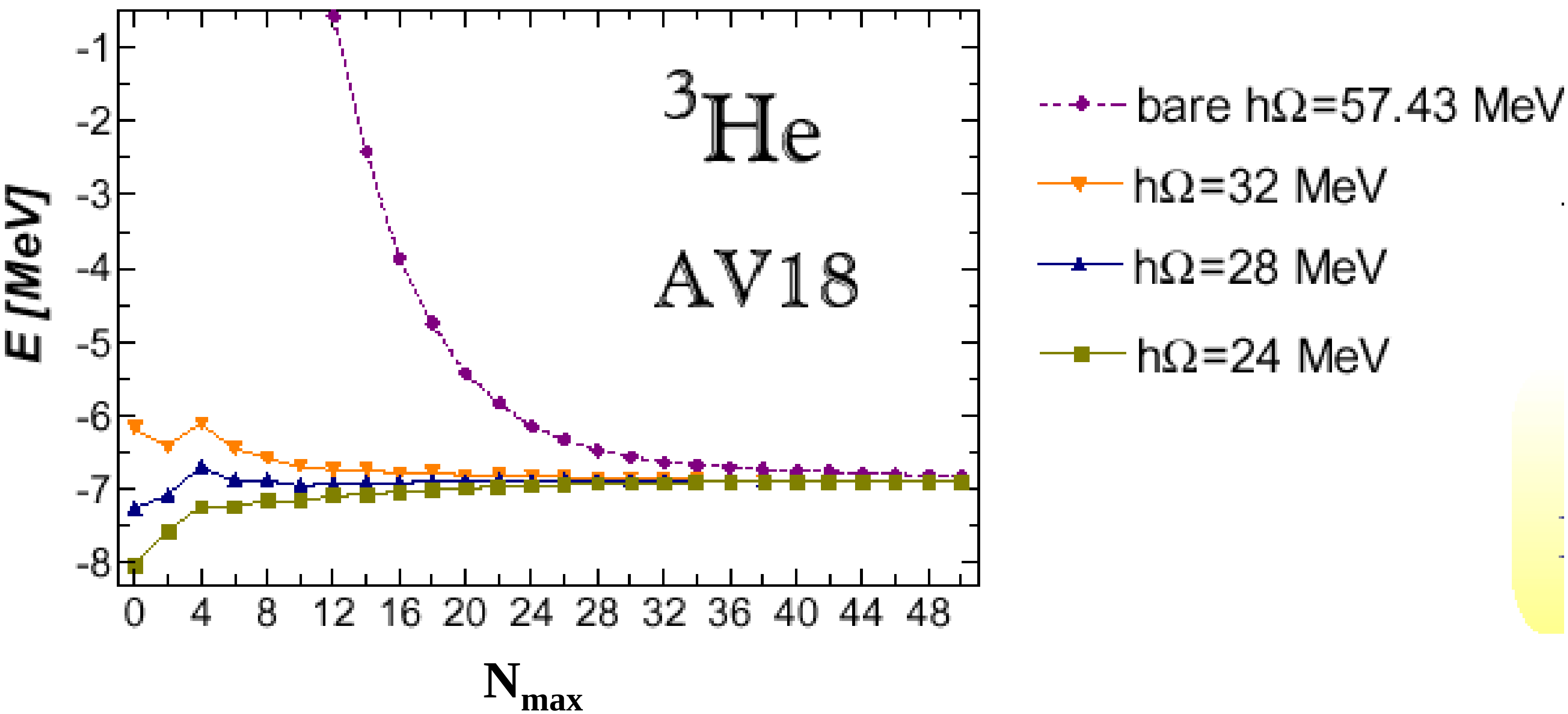
controls momentum scale limit

$\boxed{\hbar\Omega}$ controls length scale of basis functions (“box”)

Results compare well with VMC and GFMC results

Transformed system decouples low and high-momentum states

	$PH_{eff}P$ Low p nucleon modes	0
UV reg →	0	$QH_{eff}Q$ High p nucleon modes - formally retained! Quarks and gluons possible?

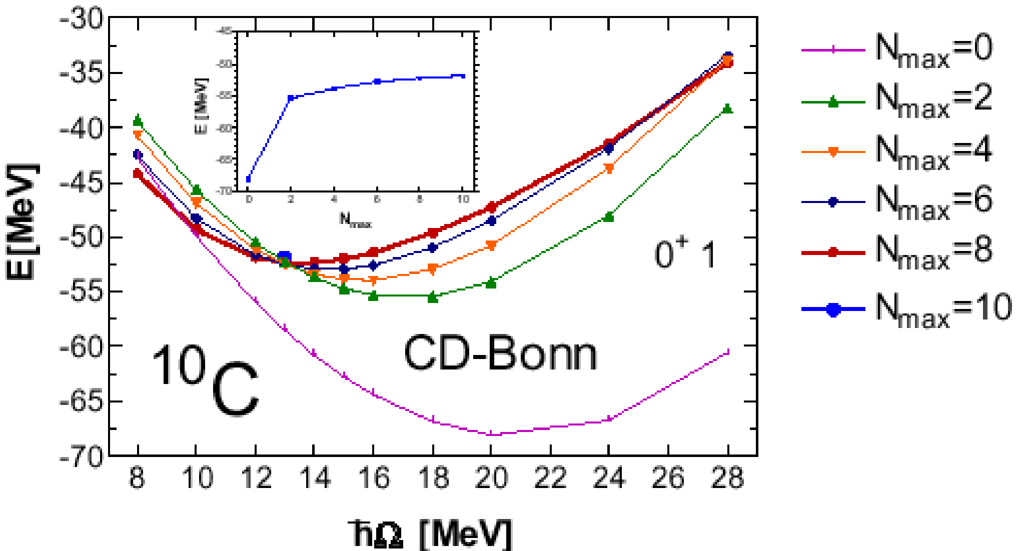


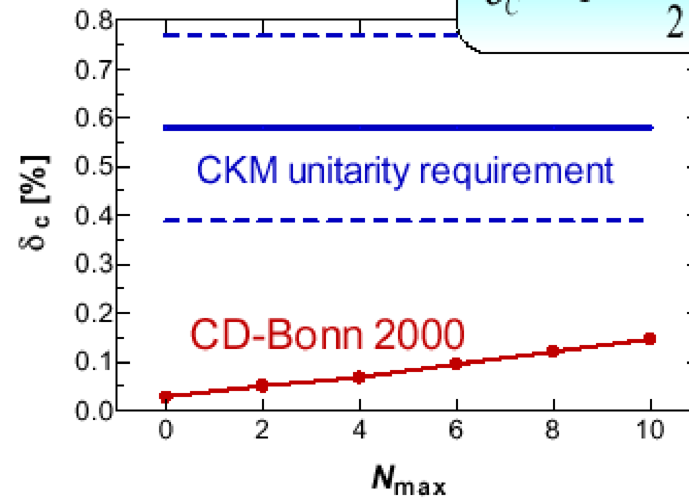
^{3}He
AV18
bare hΩ=57.43 MeV
hΩ=32 MeV
hΩ=28 MeV
hΩ=24 MeV
E [MeV]
-1
-2
-3
-4
-5
-6
-7
-8
0
4
8
12
16
20
24
28
32
36
40
44
48
N_{max}

Isospin mixing correction of $^{10}C \rightarrow {}^{10}B$ Fermi matrix element

Relevant to CKM matrix unitarity

$$\delta_C = 1 - \frac{M_F^2}{2}$$

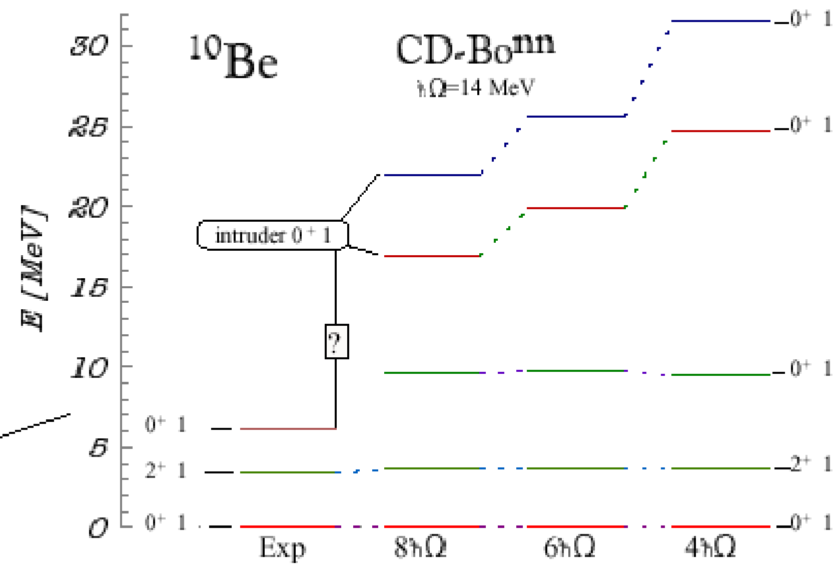




- ^{10}C and ^{10}B 0^+ 1 calculations up to $10\hbar\Omega$
  - Code Antoine (E. Caurier) - dimension 8×10^8

$$M_F = \langle {}^{10}B; 0^+1 | T_- | {}^{10}C; 0^+1 \rangle$$

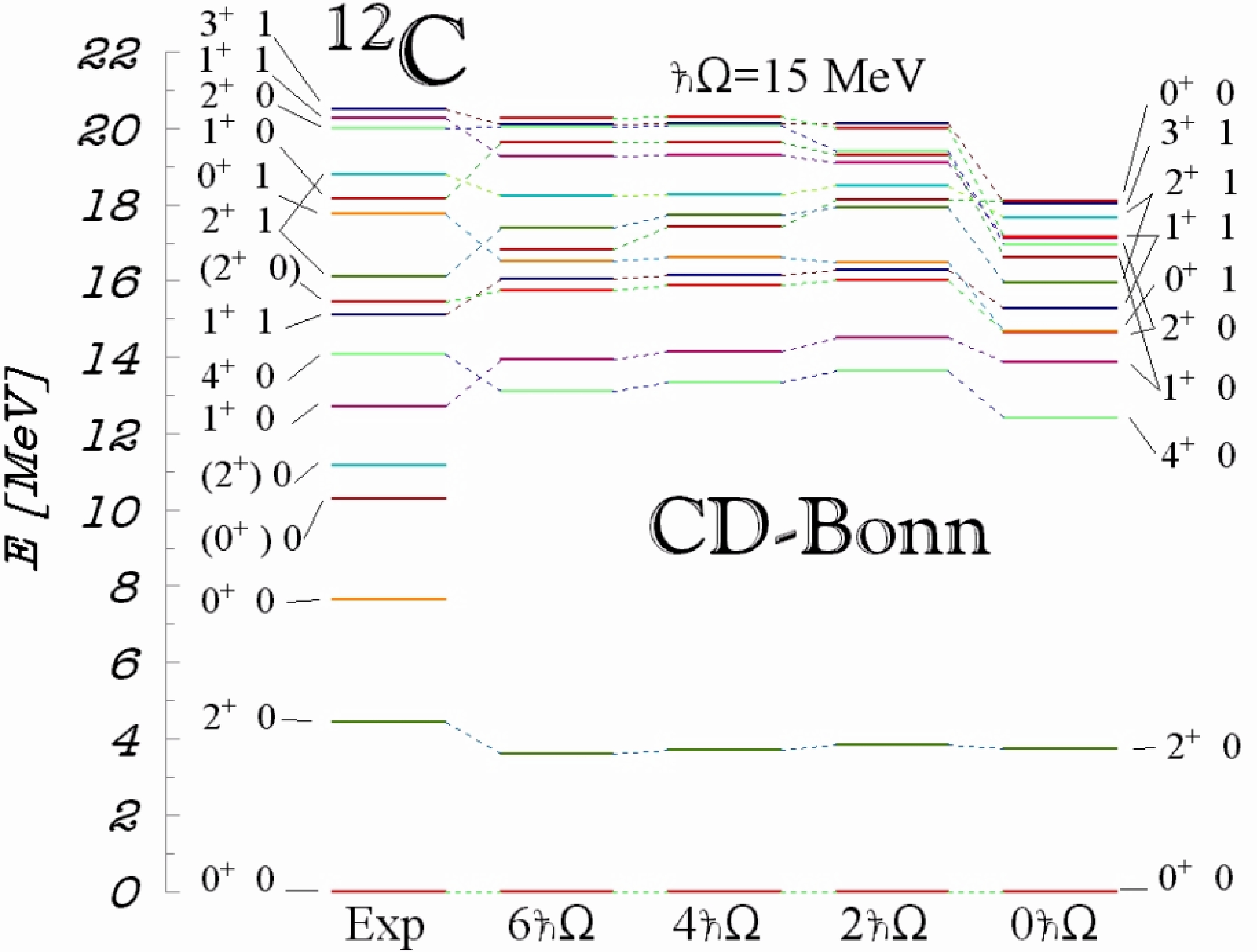
  - $=\sqrt{2}$ for an isospin invariant system
- Needed to extract v_{ud} m.e. from experimental Fermi β- decay ft values



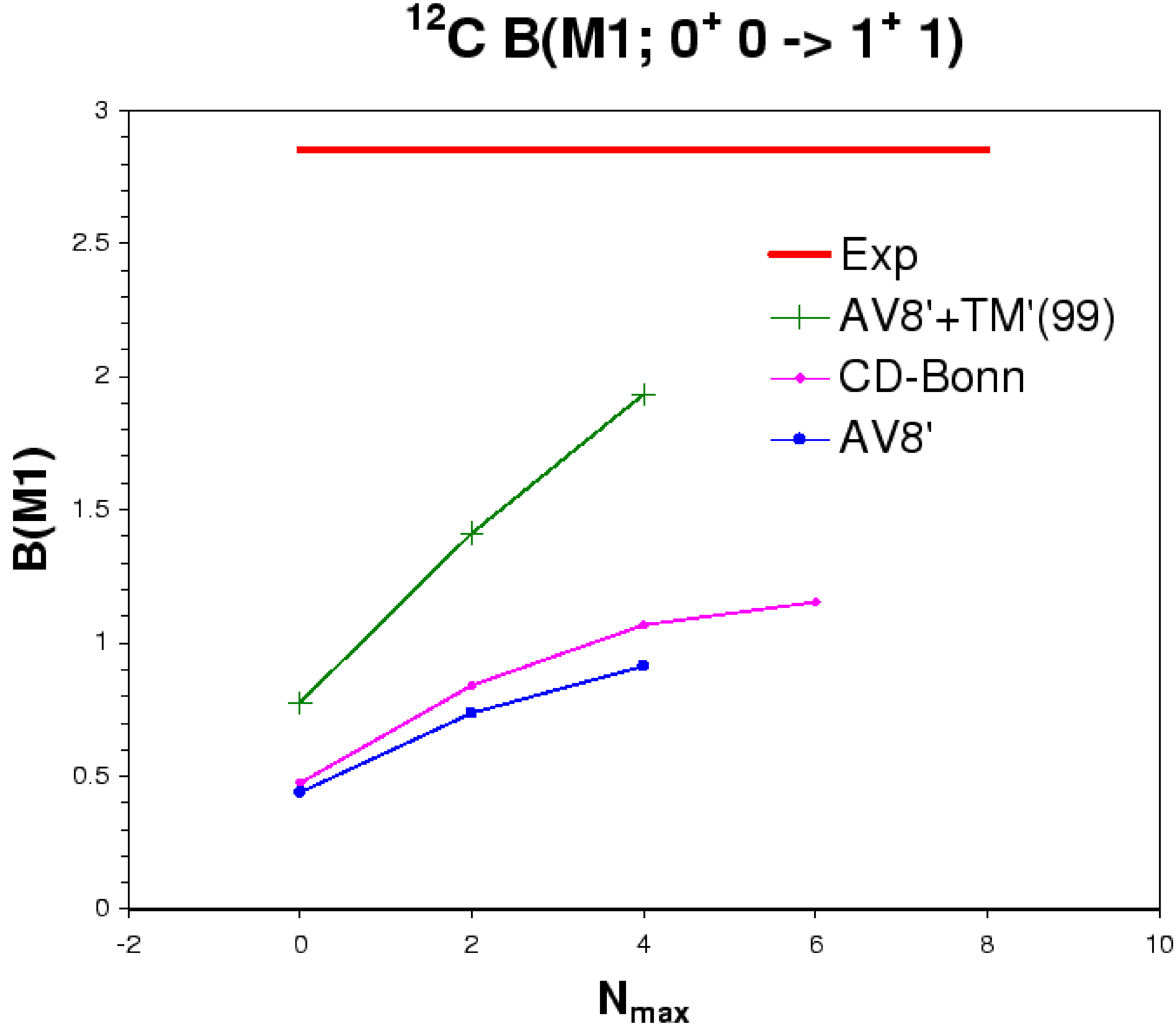
Extrapolated value: $\delta_C \approx 0.19$ %
Insufficient for CKM unitarity

Nuclear Theory & Modeling Group

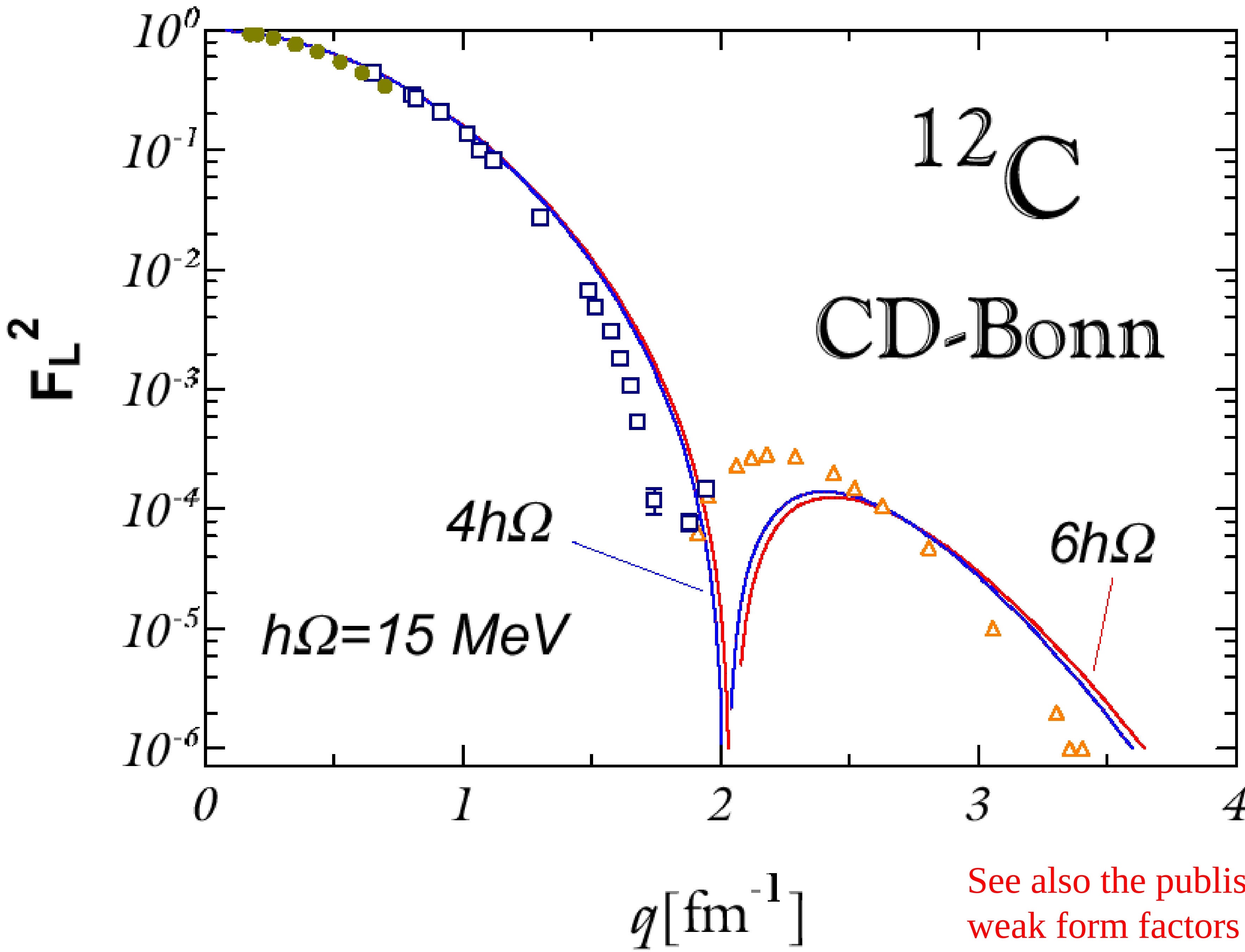
Physics & Advanced Technologies N Division



12C
ħΩ=15 MeV
CD-Bonn
E [MeV]
0
2
4
6
8
10
12
14
16
18
20
22
Exp
6ħΩ
4ħΩ
2ħΩ
0ħΩ
3+ 1
1+ 1
2+ 0
1+ 0
0+ 1
2+ 1
(2+ 0)
1+ 1
4+ 0
1+ 0
(2+) 0
(0+) 0
0+ 0
2+ 0
0+ 0
0+ 0
3+ 1
2+ 1
1+ 1
0+ 1
2+ 0
1+ 0
4+ 0
2+ 0
0+ 0

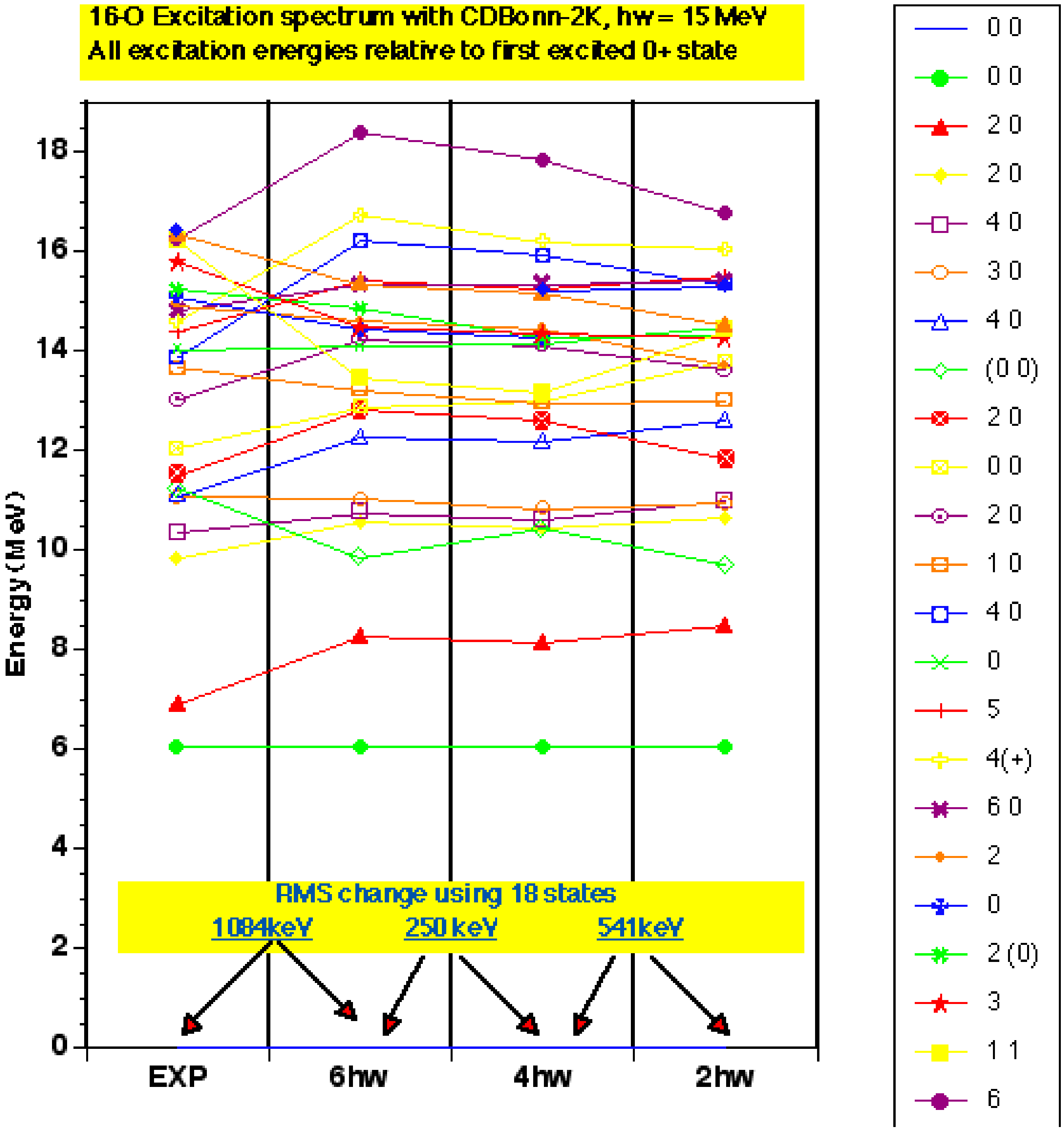


^{12}C B(M1; 0+ 0 -> 1+ 1)
B(M1)
N_{max}
Exp
AV8'+TM'(99)
CD-Bonn
AV8'
3
2.5
2
1.5
1
0.5
0
-2
0
2
4
6
8
10

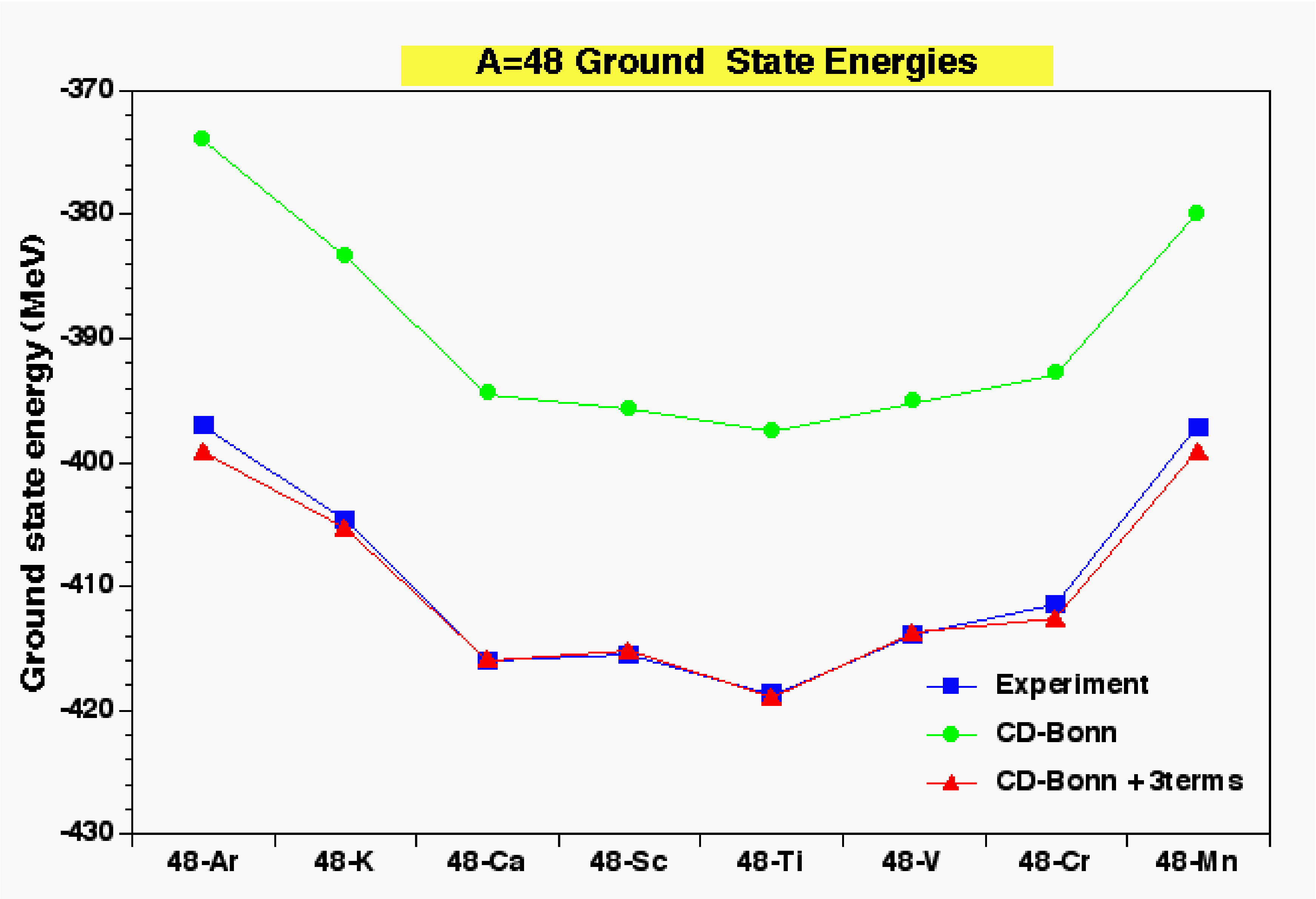


See also the published weak form factors

Results from our 16-O investigations were shown here. However, as most are not yet published, except for the one spectrum that follows, I refrain from posting them on the web.



16-O Excitation spectrum with CDBonn-2K, hw = 15 MeV
All excitation energies relative to first excited 0+ state
Energy (MeV)
18
16
14
12
10
8
6
4
2
0
EXP
6hw
4hw
2hw
RMS change using 18 states
1084keV
250 keV
541keV
0 0
0 0
2 0
2 0
4 0
3 0
4 0
(0 0)
2 0
0 0
2 0
1 0
4 0
0
5
4(+)
6 0
2
0
2 (0)
3
1 1
6


A=48 Ground State Energies
Ground state energy (MeV)
-370
-380
-390
-400
-410
-420
-430
48-Ar
48-K
48-Ca
48-Sc
48-Ti
48-V
48-Cr
48-Mn
Experiment
CD-Bonn
CD-Bonn +3terms

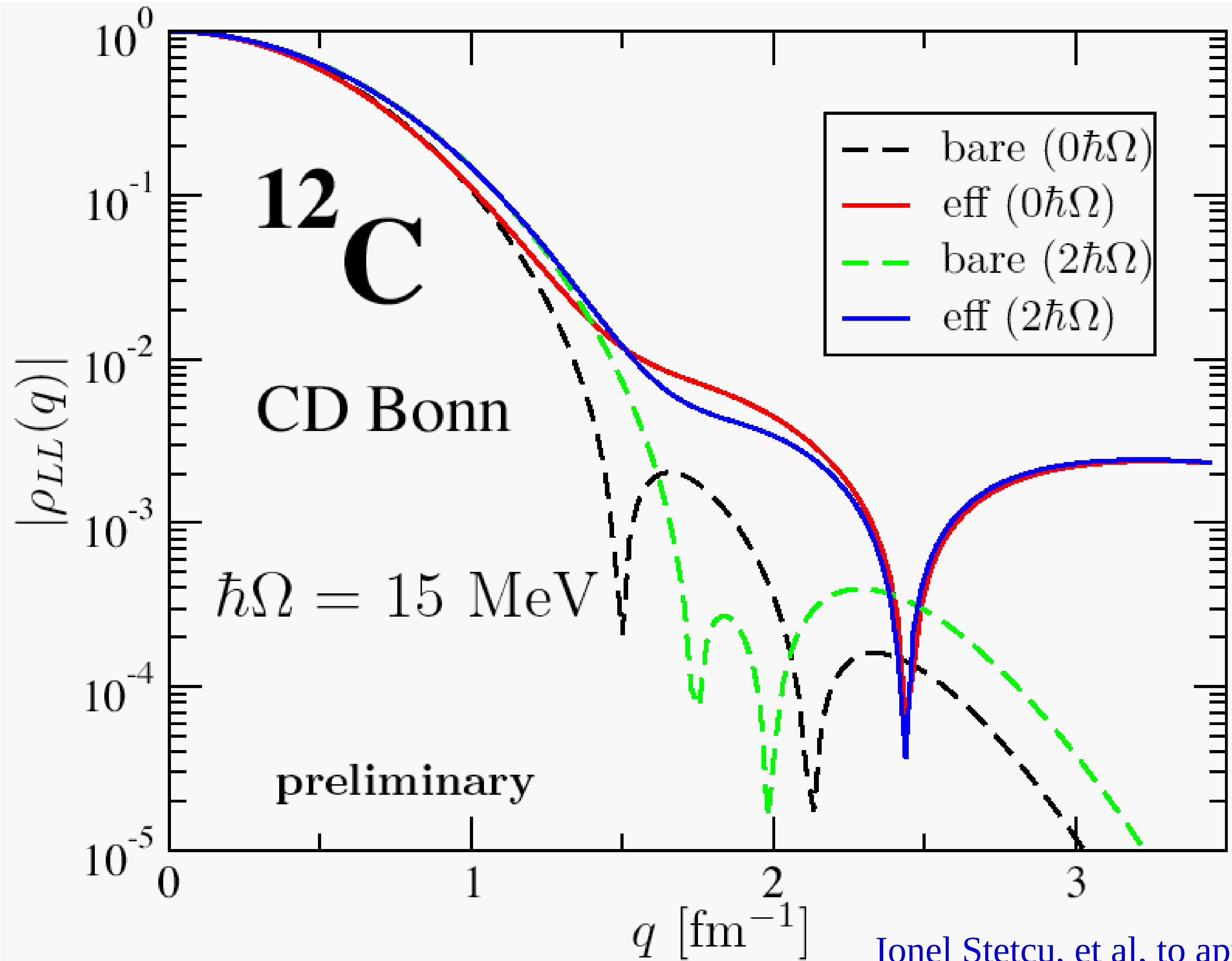
Higher energy observables

Consider the Longitudinal-Longitudinal (LL) response function, sensitive to short-range NN correlations and to our effective operator treatment. Our translational invariance is key attribute for the result.

Take simple test case - spin & isospin averaged LL response:

$$\left|\rho_{LL}(q)\right| = \left|\frac{2}{A(A-1)}\sum_{i<j}\int d^3r_i d^3r_j \left\langle \Psi_0 \right| e^{i\vec{q}\bullet(\vec{r}_i-\vec{r}_j)} \left| \Psi_0 \right\rangle\right|$$

$$= \left|\frac{2}{A(A-1)}\sum_{i<j}\int d^3r_i d^3r_j \left\langle \tilde{\Psi}_0 \right| e^{-S_a} e^{i\vec{q}\bullet(\vec{r}_i-\vec{r}_j)} e^{S_a} \left| \tilde{\Psi}_0 \right\rangle\right|$$



Ionel Stetcu, et al, to appear

How can we imagine moving to even higher momenta and energies as appropriate to JLAB with high intensity 12 GeV beams?

Return to basic theory, e.g. QCD, and start all over - <u>Hard</u>

OR

Retain the P-Q division with the dynamics in the Q-space derived in "more fundamental" degrees of freedom - <u>Hard</u>

* * * **But SJB 8/20/2004: "Just do it"** * * *

How do we use successful low-energy theory to constrain/complement higher-energy theory/experiment?

Until one of these hard problems is solved by a community-wide effort, let us examine a model, the "Quark Cluster Model" which was developed for use with NCSM wavefunctions.

Consistency requires that we work with intrinsic coordinates exploiting our translational invariance and all observables are treated as local operators - coordinate space many-body wavefunctions have a new P & Q space interpretation as shown in the following pictures.

Additional motivation comes from the uncertainty at short distances which has been integrated out in the effective Hamiltonian method

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

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TIFF (Uncompressed) decompressor
are needed to see this picture.

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TIFF (Uncompressed) decompressor
are needed to see this picture.

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Each 3q cluster is separated from another by $d < 2R_c$

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Snapshots of the A=3 probability density

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TIFF (Uncompressed) decompressor
are needed to see this picture.

Orthnormal state decomposition from configurations to single quark amplitudes:
from configurations in A=3 system:

$$p_A = \frac{A}{A+B+C}, \quad p_B = \frac{B}{A+B+C}, \quad p_C = \frac{C}{A+B+C}$$

$$\tilde{p}_3 = p_A + \frac{1}{3} p_B, \quad \tilde{p}_6 = \frac{2}{3} p_B, \quad p_9 = p_C$$

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TIFF (Uncompressed) decompressor
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We will need to update this table with the new NCSM results to make more precise comparisons with new and future JLAB data!

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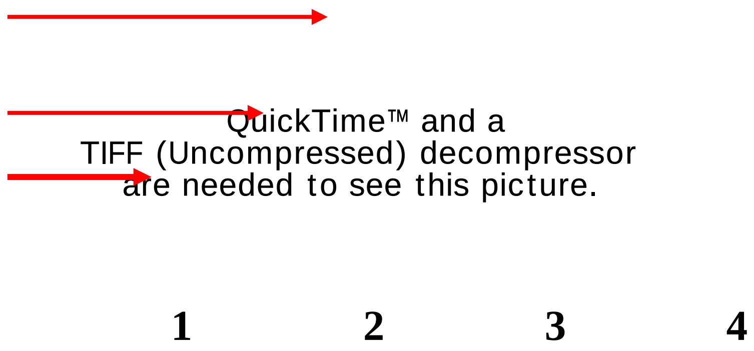
are needed to see this picture.

Signature of the Quark Cluster Model (QCM) in the scaling regime
“Steps” of ratios are simple ratios of quark cluster probabilities



Known for more than 20 years as a signature of the QCM

SLAC data - NE3

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Constituent Quark Models of Exotic Mesons

R. Lloyd, PhD Thesis, ISU 2003

Phys. Rev. D 70: 014009 (2004)

H = T + V(OGE) + V(confinement)

Solve in HO basis as a bare H problem & study dependence on cutoff

Symmetries:

Exact treatment of color degree of freedom <-- Major new accomplishment

Translational invariance preserved

Angular momentum and parity preserved

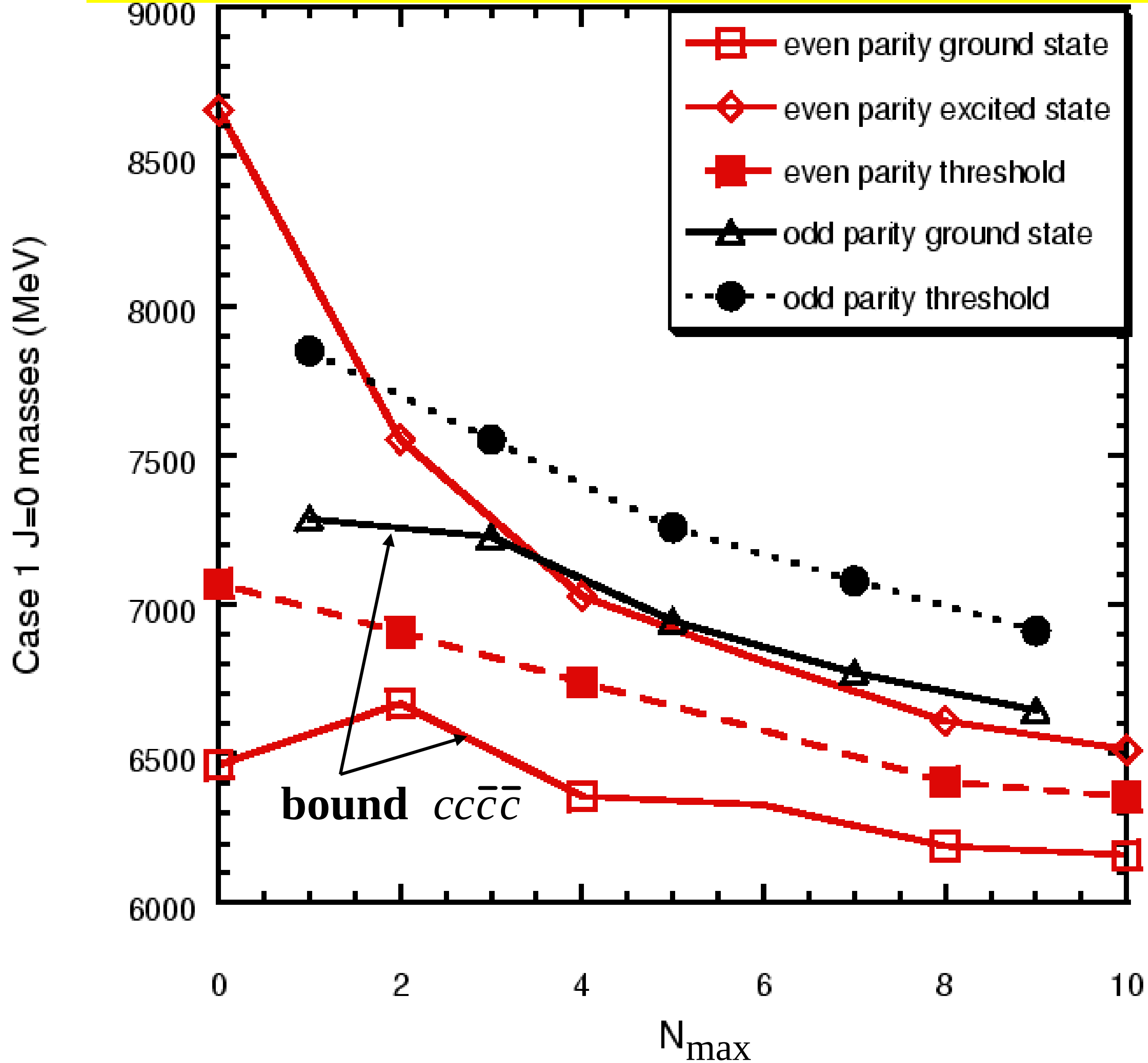
Next generation:

More realistic H fit to wider range of mesons and baryons

Beyond that generation:

H_{eff} derived from QCD

All-charm tetraquarks with bare phenomenological interaction

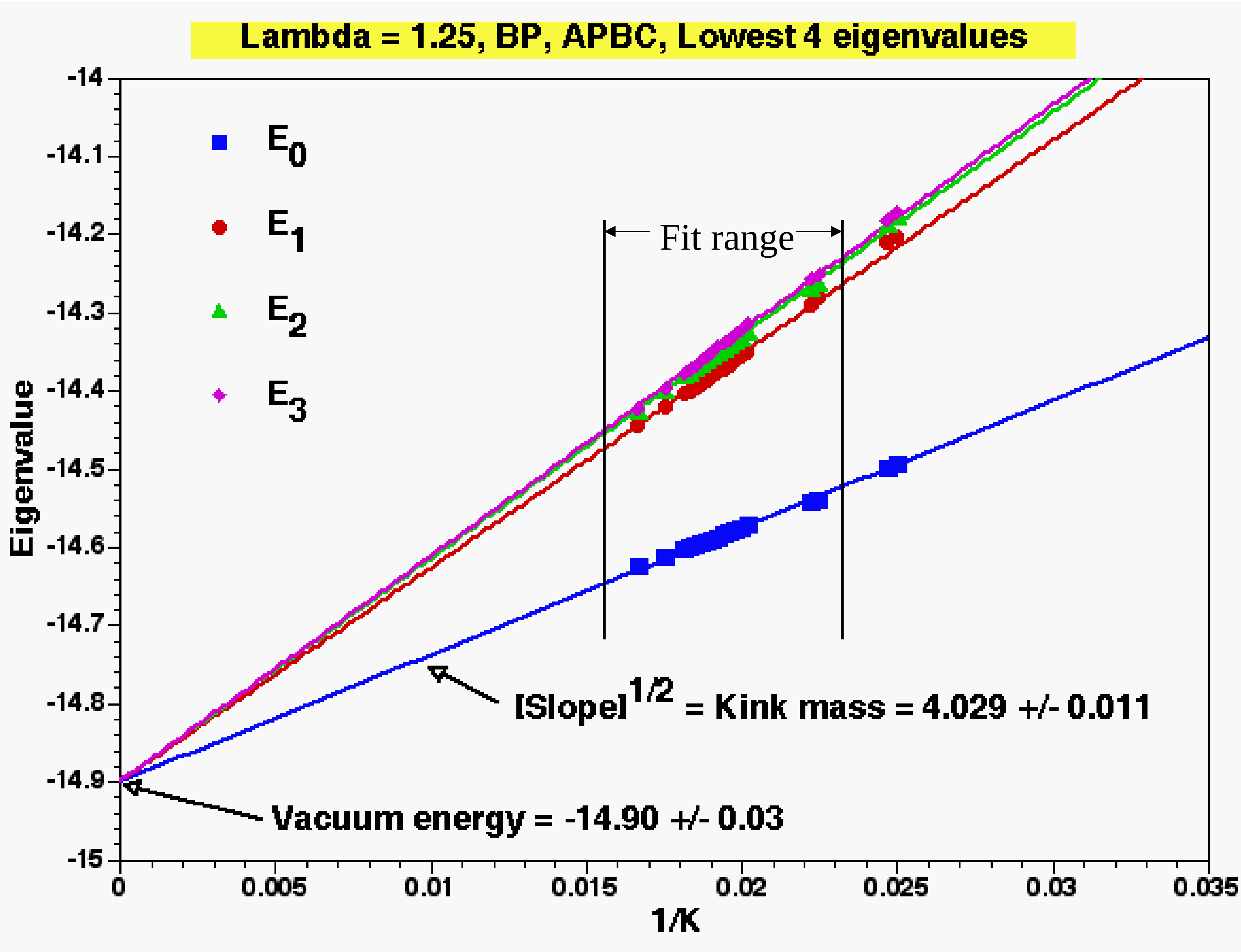


One step towards "Just do it"

Φ^4 in 1+1 Dimensions

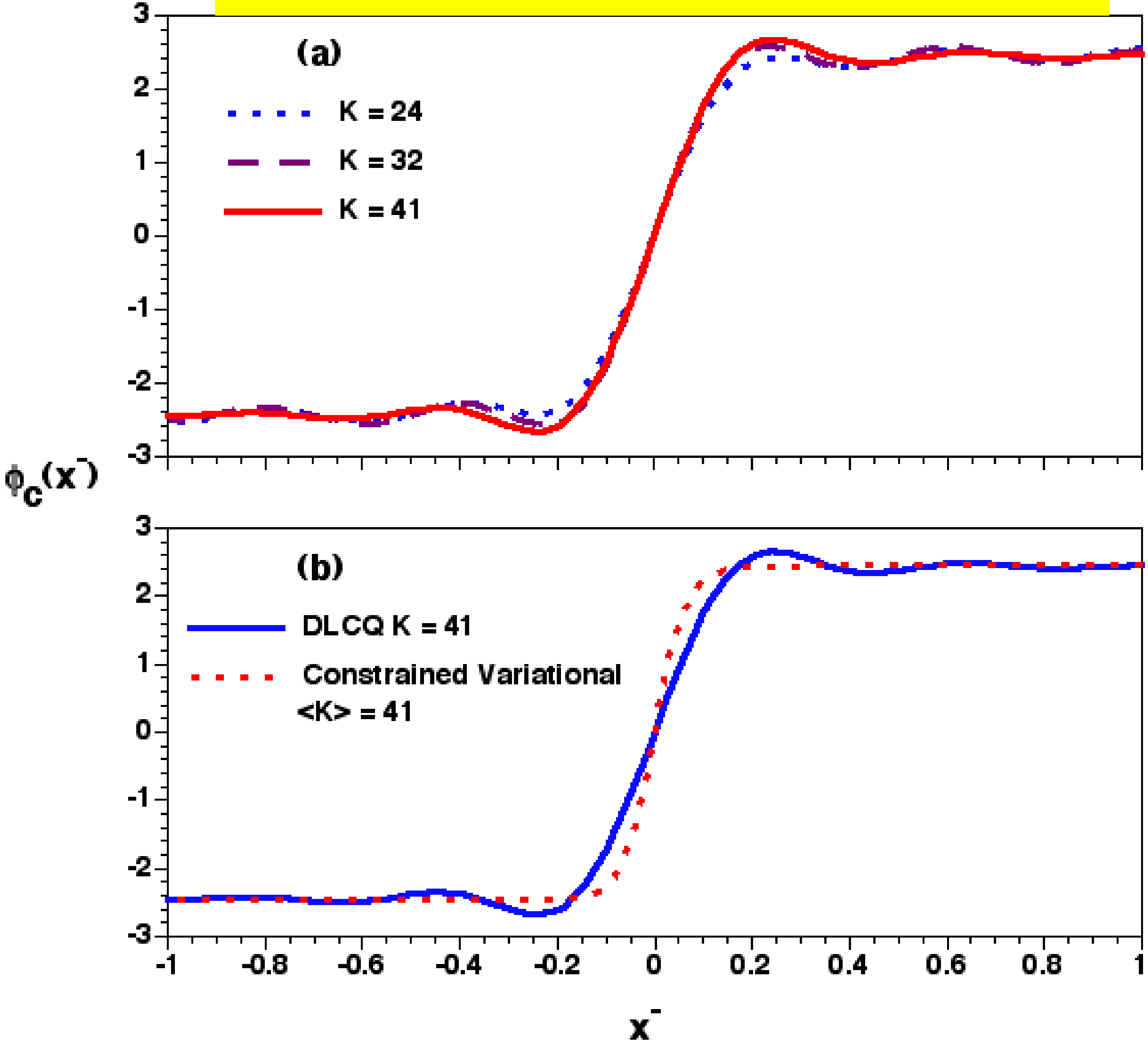
Burning issues

Demonstrate degeneracy - Spontaneous Symmetry Breaking
Topolgical features - soliton mass and profile (Kink, Kink-Antikink)
Quantum modes of kink excitation
Phase transition - critical coupling, critical exponent and
the physics of symmetry restoration
Role and proper treatment of the zero mode constraint
Chang's Duality

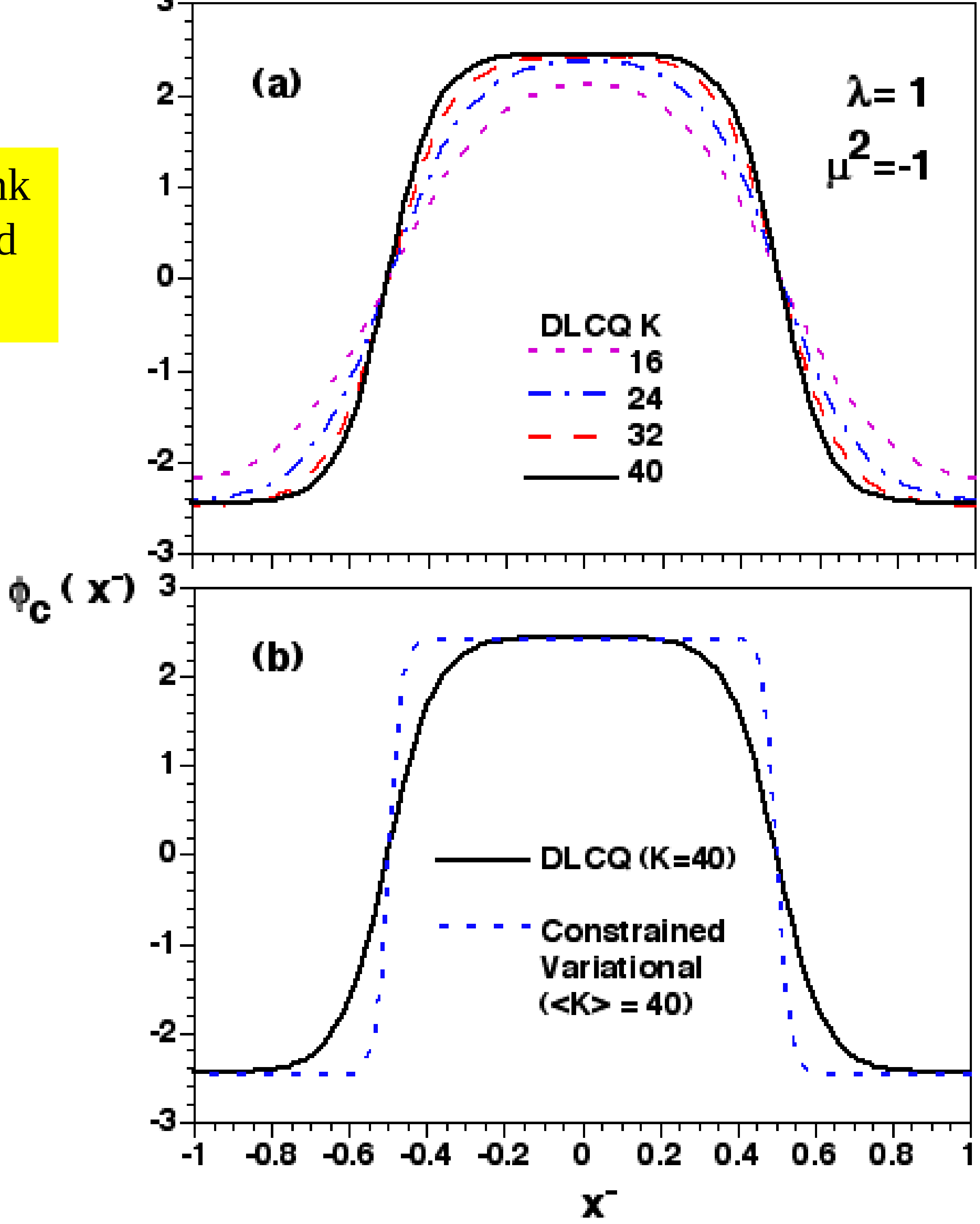


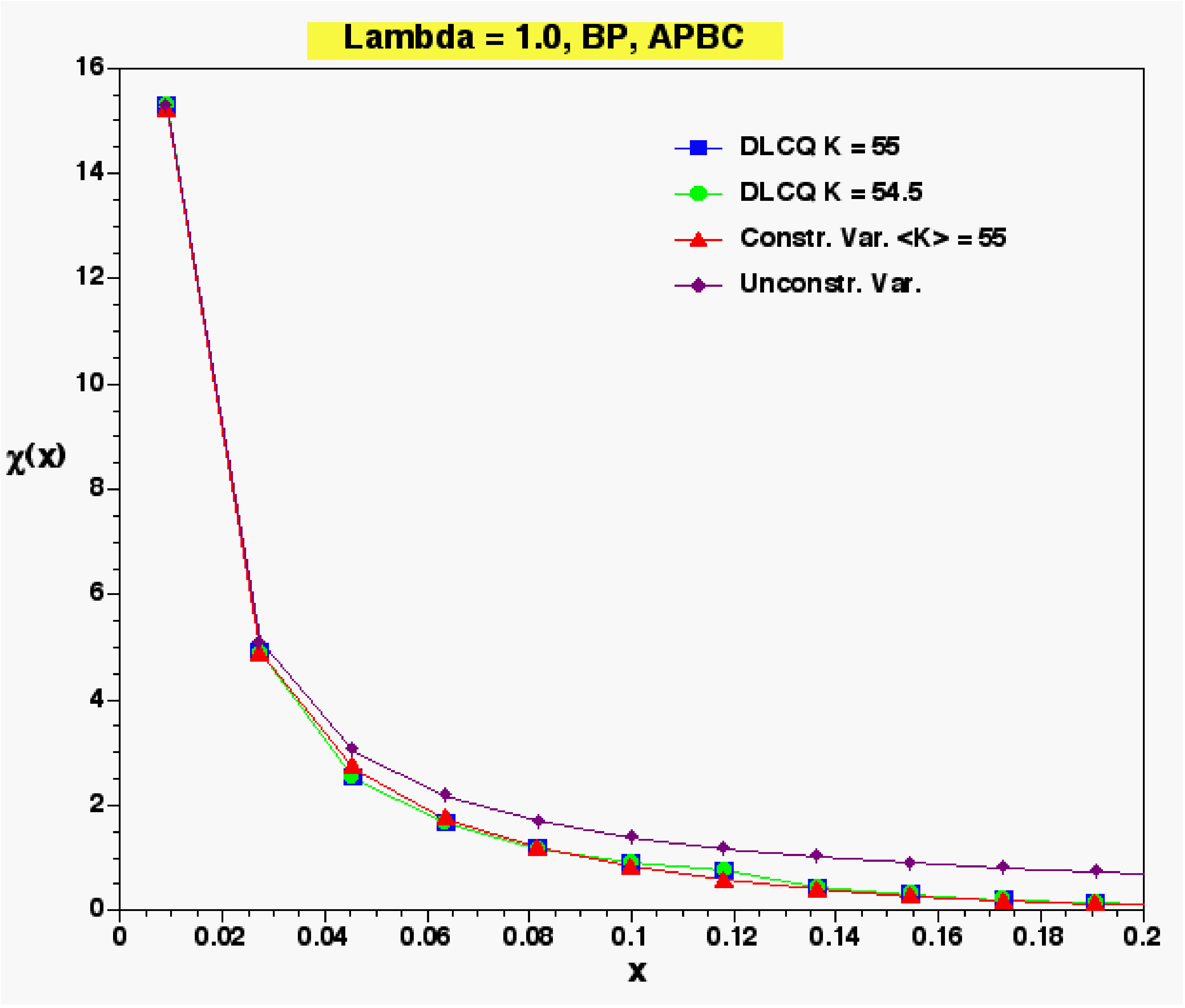
Lambda = 1.25, BP, APBC, Lowest 4 eigenvalues
Eigenvalue
1/K
E0
E1
E2
E3
Fit range
[Slope]1/2 = Kink mass = 4.029 +/- 0.011
Vacuum energy = -14.90 +/- 0.03
-14
-14.1
-14.2
-14.3
-14.4
-14.5
-14.6
-14.7
-14.8
-14.9
-15
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035

Quantum kink (soliton) in scalar field theory at $\lambda = 1$

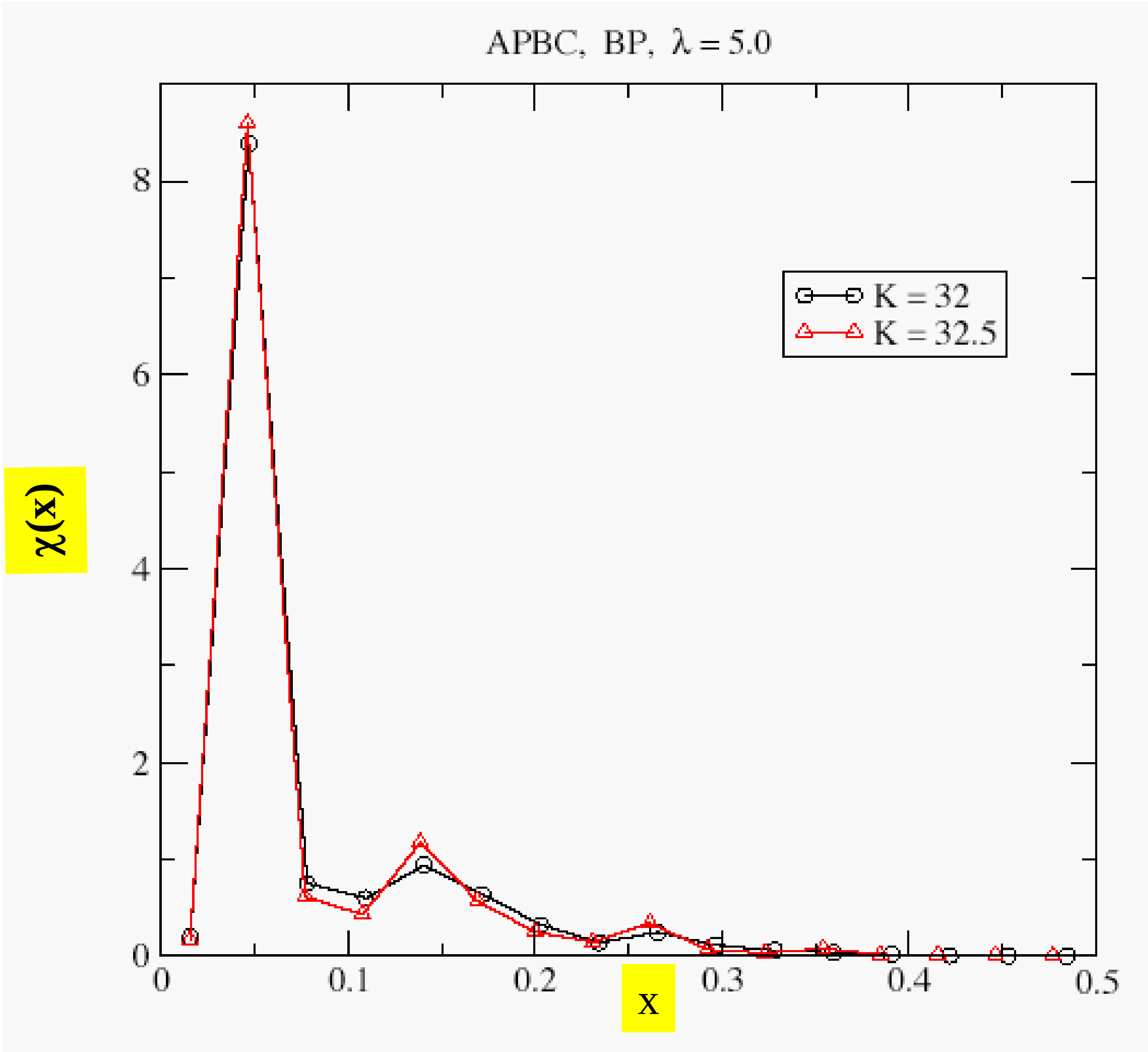


Quantum kink-antikink (soliton) in scalar field theory at $\lambda = 1$





Lambda = 1.0, BP, APBC
DLCQ K = 55
DLCQ K = 54.5
Constr. Var. <K> = 55
Unconstr. Var.
χ(x)
x
0
2
4
6
8
10
12
14
16
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2


APBC, BP, λ = 5.0
K = 32
K = 32.5
χ(x)
x
0
2
4
6
8
0
0.1
0.2
0.3
0.4
0.5

Conclusions

- **Similarity of "two-scale" problems in many-particle quantum systems**
- **Ab-initio theory is convergent exact method for solving many-particle Hamiltonians**
- **Method has been demonstrated as exact in the nuclear physics applications**
- **Realistic V_{NN}'s underbind ^{12}C 1.2 and ^{16}O by 0.5 - 1.5 MeV/A**
- **Confirm need for NNN forces to achieve high quality description of light nuclei when local NN interactions used**
- **Some advantages seen with "soft" NN interactions (V-lowk, JISP6, INOY) where ab-initio NCSM is now used to help resolve off-shell freedom**
- **First applications to heavier systems (A = 47 - 48 - 49) - new Hamiltonian**
- **Critical properties of quantum field theory emerging**
- **Posit link between ab-initio NCSM and quark cluster model (P-space ~ [$r_{ij} > 2R_c$])**
- **Advent of low-cost parallel computing has made new physics domains accessible: we have achieved a fully scalable and load-balanced algorithm.**

Outlook

With five examples - our new ability to determine:

- **Three nucleon forces**
- **v_{ud} for CKM mass matrix unitarity**
- **Majorana mass of neutrino through double β decay**
- **Critical properties of quantum field theory**
- **Foundation for a quark cluster model of nuclei**

We Have a New Physics Discovery Engine

ANNOUNCEMENT

New Tenure-Track Assistant Professor position
in Nuclear Theory at Iowa State University
(tenure track) and RIKEN Fellow position.

"Strong Interaction Theory"

Applications now being accepted

See me for details