Handling Excited States on the Lattice: The GEVP Method

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Summary

In Lattice QCD, energy levels (masses) and decay constants of quark bound states are computed from the exponential decay of Euclidean correlation functions $C(t)$, built from composite fields with the quantum numbers of the desired state.

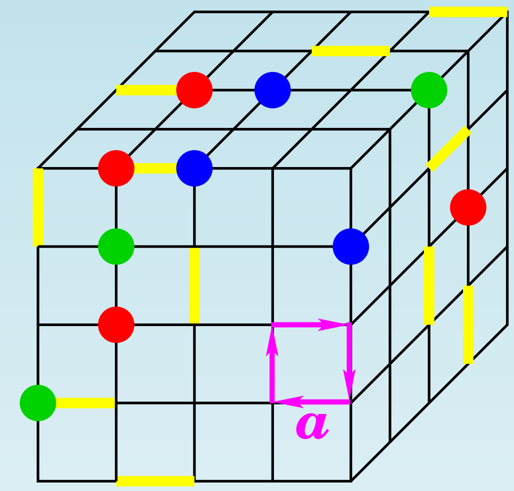
The Generalized Eigenvalue Problem (GEVP) is a valuable tool to reduce systematic errors in these determinations, and thus to deliver high-precision tests of QCD.

We derive (analytically) an optimal use of the method and demonstrate its applicability for the case of static B-mesons as well as to order $1/m$ in HQET.

Lattice QCD in a Nutshell

Three ingredients

1. Quantization by path integrals $\Rightarrow$ sum over configurations with "weights" $e^{i\,S/\hbar}$
2. Euclidean formulation (analytic continuation to imaginary time) $\Rightarrow$ weight becomes $e^{-S/\hbar}$
3. Discrete space-time $\Rightarrow$ UV cut at momenta $p \lesssim 1/a$ $\Rightarrow$ regularization



Also: finite-size lattices $\Rightarrow$ IR cut for small momenta $p \approx 1/L$

The Wilson action

$$S \;=\; \frac{\beta}{3} \sum_{\Box} \text{ReTr}\, U_{\Box}\,, \quad U_{x,\mu} \;\equiv\; e^{i g_0 a A^b_\mu(x) T_b}\,, \quad \beta \;=\; 6/{g_0}^2$$

Confinement at $\beta \approx 0$; physics corresponds to $a \to 0$...

Quark Bound States from Lattice QCD

The recipe for lattice simulations:

1) Evolve gluon fields (link variables) in the Monte Carlo dynamics associated with the partition function

$$Z \;=\; \int \mathcal{D}U \, e^{-S_g} \int \mathcal{D}\psi \, \mathcal{D}\overline{\psi} \;\, e^{-\int d^4x \; \overline{\psi}(x) \; K \; \psi(x)} \;=\; \int \mathcal{D}U \, e^{-S_g} \; \det K(U)$$

(the quenched approximation corresponds to $\det K = 1$)

2) Obtain quark propagators from $< \psi \, \overline{\psi} > = < K^{-1} >$

3) Use the "quark fields" to build (Euclidean) correlators for the desired bound states $C(t) \; = < O(t) \, O(0) >$, where $O(t) = \overline{\psi} \, \Gamma \, \psi$ and Γ is the appropriate Dirac matrix (e.g. $\Gamma = \gamma_5$ for pseudoscalar mesons)

4) Extract masses, etc from $C(t) \; \rightarrow \; \sum_n |< 0|O|n >|^2 \, e^{-E_n t}$
$\Rightarrow$ at large t $\;\; m_{eff}(t) = \log[C(t)/C(t+1)]$ approaches a plateau

5) Translate to physical units: e.g. $m = m_{latt}/a$ (then take $a \rightarrow 0$).

Fits of Effective Masses

Determining masses etc. from the correlators

$$C(t) \;=\; < O(t)\, O(0) > \;=\; \sum_{n=1}^{\infty} \left| < 0 |\, \hat{O} \,| n > \right|^2 e^{-E_n t}$$

is not an easy task!

Look for a plateau (at large t) in

$$E_1^{\text{eff}}(t) \;=\; \log[C(t)/C(t+1)] \;\longrightarrow\; E_1 \,+\, \mathrm{O}(\mathrm{e}^{-(E_2-E_1)t})$$

Signal competes with noise at $t \gtrsim$ 1 fm.

Multiple-exponential fits subject to large systematic errors.

Alternatives: more sophisticated fitting (Bayesian fitting, evolutionary fitting, black-box method)

Energies and Matrix Elements: GEVP

Instead of simple point sources $\Rightarrow$ all-to-all propagators, then combine different (linearly independent) interpolators, e.g. from different smearing levels, to get matrix of correlators

$$C_{ij}(t) \;=\; \langle O_i(0) O_j(t) \rangle \;=\; \sum_{n=1}^{\infty} \mathrm{e}^{-E_n t} \psi_{ni} \psi_{nj} \,, \quad i, j = 1, \ldots, N$$

$$\psi_{ni} \;\equiv\; (\psi_n)_i \;=\; \langle n | \hat{O}_i | 0 \rangle \;, \quad \langle m | n \rangle \;=\; \delta_{mn} \,.$$

Diagonalizing $C(t)$ provides estimates for energy levels E_n, through the eigenvalues $\lambda_n(t) \approx \mathrm{e}^{-E_n\, t}$. It is advantageous to solve, instead, the GEVP

$$C(t)\, v_n(t, t_0) \;=\; \lambda_n(t, t_0)\, C(t_0)\, v_n(t, t_0) \,,$$

where $t > t_0$.

Convergence

At large t get effective energy levels from $\lambda_n(t, t_0)$ as

$$E_n^{\text{eff}}(t, t_0) \;\equiv\; \log \frac{\lambda_n(t, t_0)}{\lambda_n(t+1, t_0)} \;.$$

Lüscher and Wolff, 1990: $E_n^{\text{eff}}(t, t_0)$ converges as $t \to \infty$ (and fixed t_0) to true energy E_n as

$$E_n^{\text{eff}}(t, t_0) \;=\; E_n \,+\, \mathrm{O}(\mathrm{e}^{-\Delta E_n\, t})\,, \quad \Delta E_n = \min_{m \neq n} |E_m - E_n|\,.$$

Possible large corrections if there is an energy level close to E_n, advantage of larger basis (i.e. large N) is not evident.

Initially, method applied with small t_0 (1 or 0), but better results reported for large t_0.

Efficient GEVP

Note that truncated problem (only N levels) given exactly by true energies: $\lambda_n^{(0)}(t,t_0) = \mathrm{e}^{-E_n(t-t_0)}$. Also, have $\hat{\mathcal{A}}_n$ s.t. $|n\rangle = \hat{\mathcal{A}}_n^\dagger |0\rangle$.

Perturbation theory applied to truncated problem (large t, t_0), get corrections to large-time behavior of energies and matrix elements (Blossier et al., JHEP 2009).

$$E_n^{\mathrm{eff}}(t,t_0) \;=\; E_n \,+\, \varepsilon_n(t,t_0)$$

$$\mathrm{e}^{-\hat{H}t}(\hat{\mathcal{Q}}_n^{\mathrm{eff}}(t,t_0))^\dagger|0\rangle \;=\; |n\rangle \,+\, \sum_{n'=1}^{\infty} \pi_{nn'}(t,t_0)\,|n'\rangle\,,$$

where

$$\hat{\mathcal{A}}_n^{\mathrm{eff}}(t,t_0) \;=\; \mathrm{e}^{-\hat{H}t}\hat{\mathcal{Q}}_n^{\mathrm{eff}}(t,t_0) \;=\; \mathrm{e}^{-\hat{H}t}R_n\left(\hat{O}\,,\,v_n(t,t_0)\,\right),$$

$$R_n \;=\; \left(v_n(t,t_0)\,,\,C(t)\,v_n(t,t_0)\right)^{-1/2}\,\left[\frac{\lambda_n(t_0+1,t_0)}{\lambda_n(t_0+2,t_0)}\right]^{t/2}\,.$$

Efficient GEVP (II)

Two regimes

- $t > 2t_0$: 2nd-order corrections dominate (small gap $E_m - E_n$)
- $t \leq 2t_0$: 1st-order dominates, large gap $E_{N+1} - E_n$

Amplitudes $\pi_{nn'}(t, t_0)$ get main contributions at first order.

Thus, for $t \leq 2t_0$ (and defining $\Delta E_{m,n} = E_m - E_n$)

$$\varepsilon_n(t, t_0) = \mathrm{O}(\mathrm{e}^{-\Delta E_{N+1,n}\, t})$$

$$\pi_n(t, t_0) = \mathrm{O}(\mathrm{e}^{-\Delta E_{N+1,n}\, t_0}), \quad \text{fixed } t - t_0$$

Main result is appearance of large gaps $\Delta E_{N+1,n}$.

For example, in static-light systems $\Delta E_{6,1} \approx 2$ GeV means a gain of roughly a factor of 5 in time separation.

Application to Effective Theory

In an effective theory, correlation functions

$$C_{ij}(t) \;=\; C_{ij}^{\rm stat}(t) \,+\, \omega\, C_{ij}^{1/{\rm m}}(t) \,+\, {\rm O}(\omega^2)$$

are computed in an expansion in a small parameter ω. Following the same procedure as above, we get similar suppressions for first-order corrections in an effective theory, with the energy differences of the lowest-order theory. We arrive at

$$E_n^{\rm eff}(t,t_0) \;=\; E_n^{\rm eff,stat}(t,t_0) + \omega E_n^{\rm eff,1/m}(t,t_0) + {\rm O}(\omega^2)$$

with

$$E_n^{\rm eff,stat}(t,t_0) \;=\; E_n^{\rm stat} \,+\, \beta_n^{\rm stat}\, {\rm e}^{-\Delta E_{N+1,n}^{\rm stat}\, t} + \ldots\,,$$

$$E_n^{\rm eff,1/m}(t,t_0) \;=\; E_n^{1/{\rm m}} + [\,\beta_n^{1/{\rm m}} - \beta_n^{\rm stat}\, t\, \Delta E_{N+1,n}^{1/{\rm m}}\,]{\rm e}^{-\Delta E_{N+1,n}^{\rm stat}\, t} + \ldots\,.$$

and similarly for matrix elements.

(Lattice) Heavy-Quark Effective Theory

Presently no lattice is large enough to describe simultaneously the two scales of B-physics: $\Lambda_{\rm QCD}$ and the b-quark mass.

$\Rightarrow$ (lattice) HQET, valid low-momentum description, manifest heavy-quark symmetry for $m_b \to \infty$ (static Lagrangian)

$$\mathcal{L}^{\rm HQET} \;=\; \overline{\psi}_h(x)\, D_0\, \psi_h(x) \,-\, \omega_{\rm kin}\, \mathcal{O}_{\rm kin} \,-\, \omega_{\rm spin}\, \mathcal{O}_{\rm spin}$$

where

$$\mathcal{O}_{\rm kin} \;=\; \overline{\psi}_h(x)\, \mathbf{D}^2\, \psi_h(x)\,, \qquad \mathcal{O}_{\rm spin} \;=\; \overline{\psi}_h(x)\, \sigma \cdot \mathbf{B}\, \psi_h(x)\,.$$

The parameters $\omega_{\rm kin}$ and $\omega_{\rm spin}$ break respectively the heavy-quark flavor and spin symmetries, giving the first-order (i.e. order $1/m_b$) corrections to the static Lagrangian.

Lattice HQET (II)

Thus, we have a theoretically clean solution

- start from the static approximation (describing the asymptotics as $m_b \to \infty$)
- corrections $\mathrm{O}(1/m_b)$ computed by a $1/m_b$ expansion of the statistical weight $\Rightarrow$ higher dimensional interaction terms in the effective Lagrangian treated as insertions into static correlation functions

Guarantees existence of the continuum limit and results are independent of the regularization. The theory requires non-perturbative renormalization, which can be achieved as described below

Lattice HQET (II)

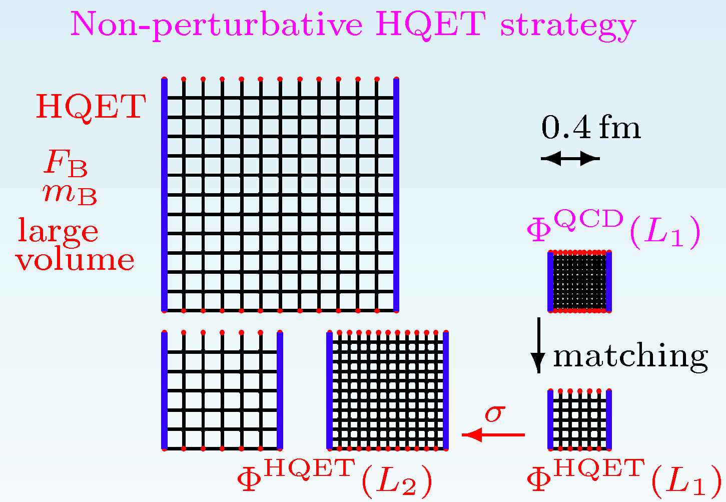
Masses and decay constants are given respectively by

$$m_B = m_{\rm bare} + E^{\rm stat} + \omega_{\rm kin} E^{\rm kin} + \omega_{\rm spin} E^{\rm spin}$$

$$f_B \sqrt{\frac{m_B}{2}} = Z_A^{\rm HQET} p^{\rm stat} (1 + c_A^{\rm HQET} p^{\delta A} + \omega_{\rm kin} p^{\rm kin} + \omega_{\rm spin} p^{\rm spin}) ,$$

where parameters $m_{\rm bare}$ and $Z_A^{\rm HQET}$ contain static and $1/m$ contributions, and $c_A^{\rm HQET}$ is also of order $1/m_b$.

Divergences cancelled in NPR procedure (Heitger and Sommer JHEP 2004), matching HQET to QCD on small lattices (in SF scheme) and extrapolation by the step-scaling method.



Nonperturbative HQET Parameters

Analysis for NP (quenched) HQET parameters recently completed: Blossier et al., arXiv:1001.4783 [hep-lat]

static coefficients for HYP2 action, at physical b-quark mass

β	$a\, m_{\rm bare}^{\rm stat}$	$\log Z_A^{\rm stat}$	$\log Z_V^{\rm stat}$
6.02190	2.043 ± 0.003	-0.062 ± 0.004	-0.040 ± 0.004
6.28850	1.325 ± 0.002	-0.099 ± 0.004	-0.077 ± 0.004
6.49560	0.970 ± 0.002	-0.116 ± 0.004	-0.094 ± 0.004

similarly, at $1/m$ order

β	$a\, m_{\rm bare}^{\rm 1/m}$	$\log Z_A^{\rm 1/m}$	$c_A^{\rm HQET}/a$	$\log Z_V^{\rm 1/m}$	$c_V^{\rm HQET}/a$
6.02190	-0.217 ± 0.007	0.04 ± 0.02	-0.33 ± 0.08	0.14 ± 0.02	0.07 ± 0.080
6.28850	-0.270 ± 0.007	0.06 ± 0.03	-0.53 ± 0.13	0.18 ± 0.02	0.12 ± 0.119
6.49560	-0.322 ± 0.008	0.07 ± 0.04	-0.70 ± 0.17	0.21 ± 0.03	0.18 ± 0.156

Nonperturbative HQET Parameters (II)

Similarly for the $\mathcal{O}(1/m)$ parameters in the HQET Lagrangian

β	$\omega_{\rm kin}/a$	$\omega_{\rm spin}/a$
6.02190	0.321 ± 0.008	0.539 ± 0.029
6.28850	0.425 ± 0.010	0.704 ± 0.039
6.49560	0.536 ± 0.013	0.858 ± 0.046

NOTE: small (but correlated) errors, expected behavior with a

$\Rightarrow$ Simulate lattice HQET, compute observables of interest, perform NP renormalization with above parameters. Since parameters are so precise, should also deliver high precision for (bare) quantities computed in the simulation!

Test of B_s-mesons in quenched HQET

- HYP1, HYP2 static quark, NP $\mathrm{O}(a)$-improved-Wilson strange quark.
- Space-time is $L^3 \times 2L$ with PBC, $L \approx 1.5$ fm, lattice spacings: 0.1 fm, 0.07 fm and 0.05 fm.
- All-to-all strange-quark propagators constructed from (approximate) low modes, 100 configurations.
- APE smearing for gauge links in interpolators, Gaussian smearing (8 levels) for strange-quark field.
- Simple $\gamma_0\gamma_5$ structure in Dirac space for all 8 interpolating fields.
- Local field (no smearing) included to compute the decay constant.

Choice of Interpolator Basis

The resulting (8×8) correlation matrix may be conveniently truncated to an $N \times N$ one, then GEVP is solved for each N and results can be studied as a function of N.

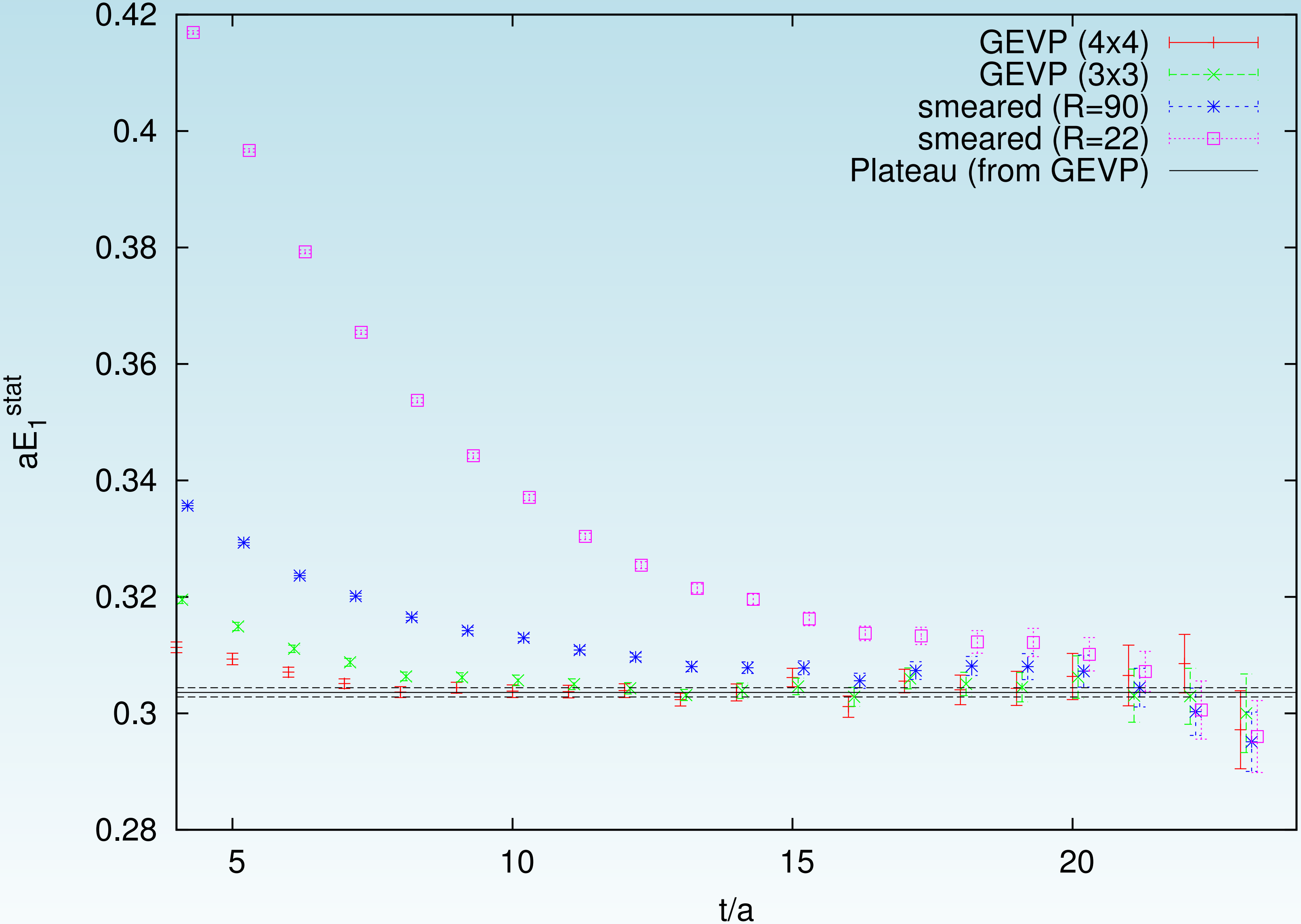
Did first analysis by projecting (at $t_i \approx$ 0.2 fm) with the N eigenvectors of $C(t_i)$ with the largest eigenvalues

$$C(t_i)\, b_n = \lambda_n\, b_n \quad \Rightarrow \quad C^{(N\times N)}_{nm}(t) \;=\; b_n^\dagger\, C(t)\, b_m\,, \quad n, m \le N\,.$$

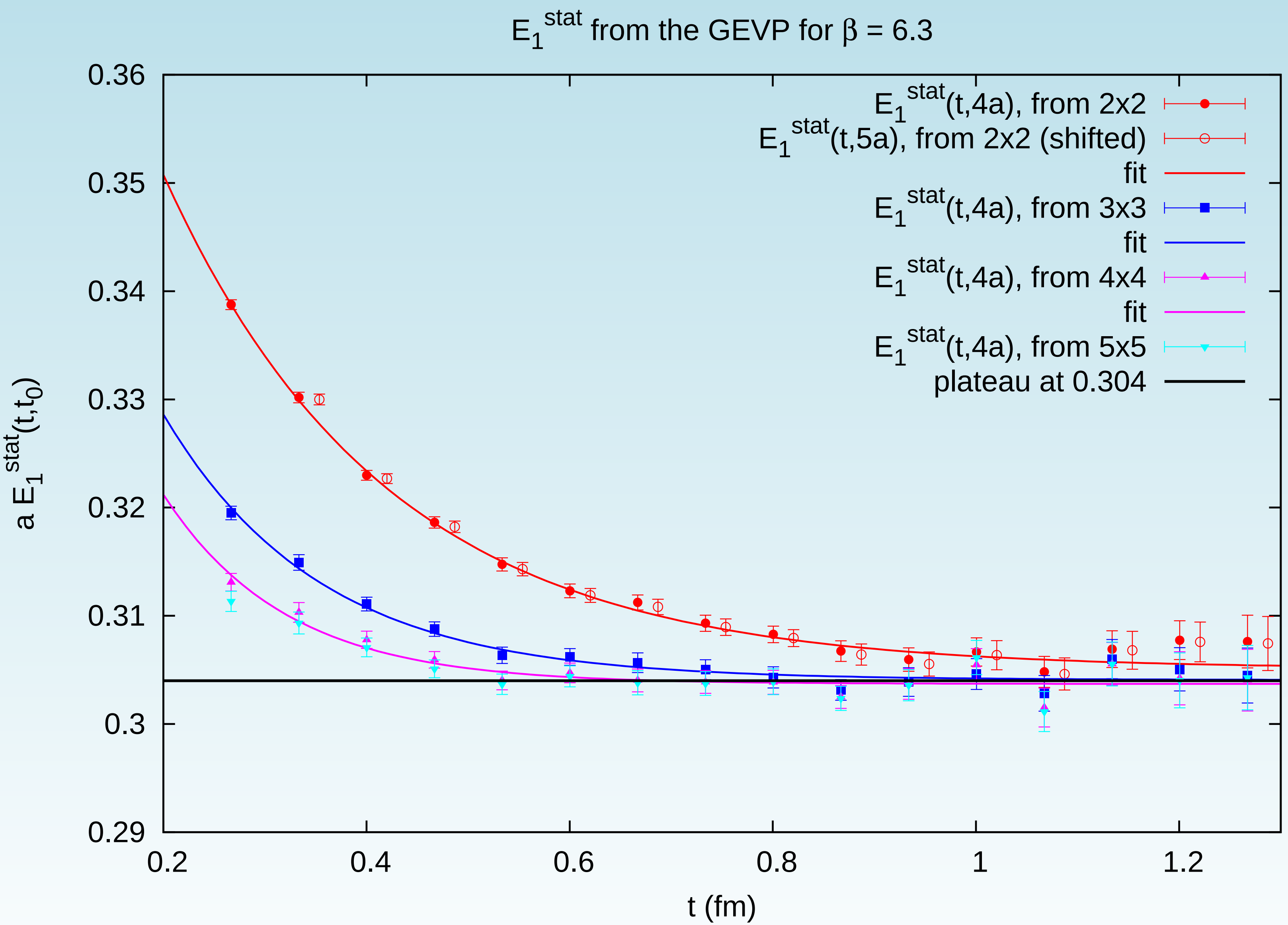
Strong dependence on N, see that $N = 2$ is not safe.

Then picked basis from unprojected interpolators, sampling the different smearing levels (from 1 to 7) as $\{1,7\}$,$\{1,4,7\}$ etc. Get better plateaus, weaker dependence on N for ground-state energies. Results remain unchanged.

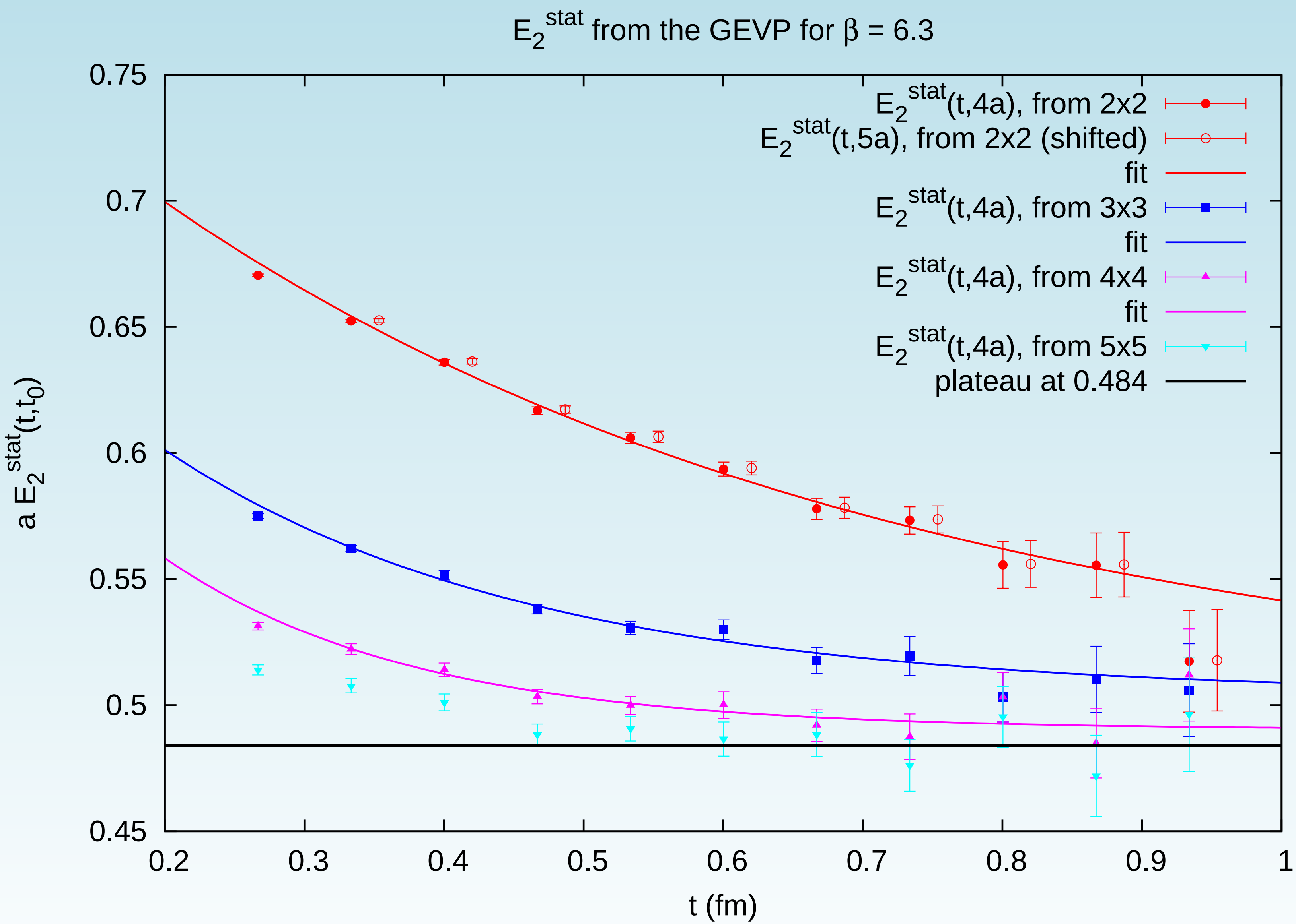
Efficiency of the Method



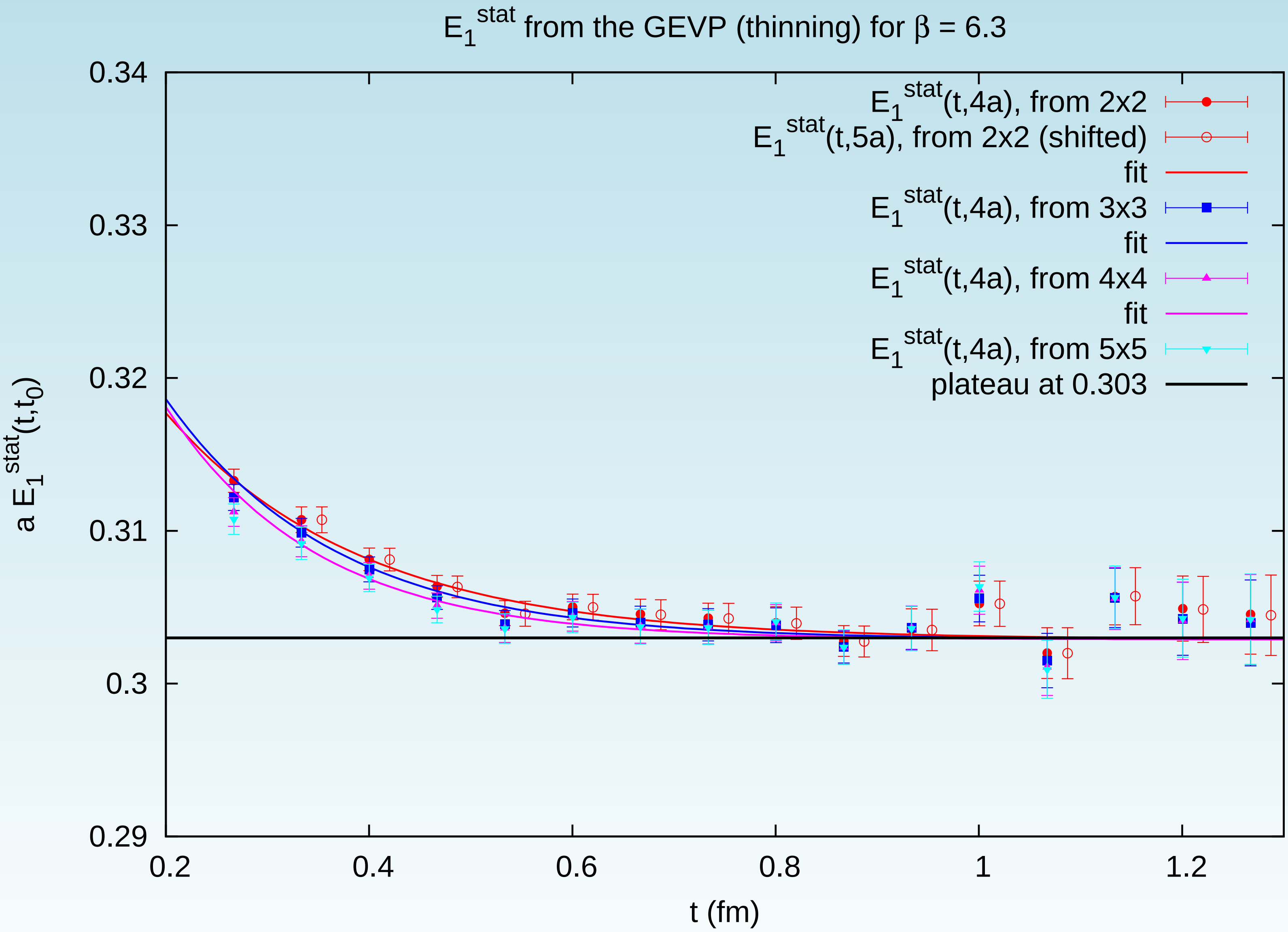
Spectrum: Static Energy, 1st basis



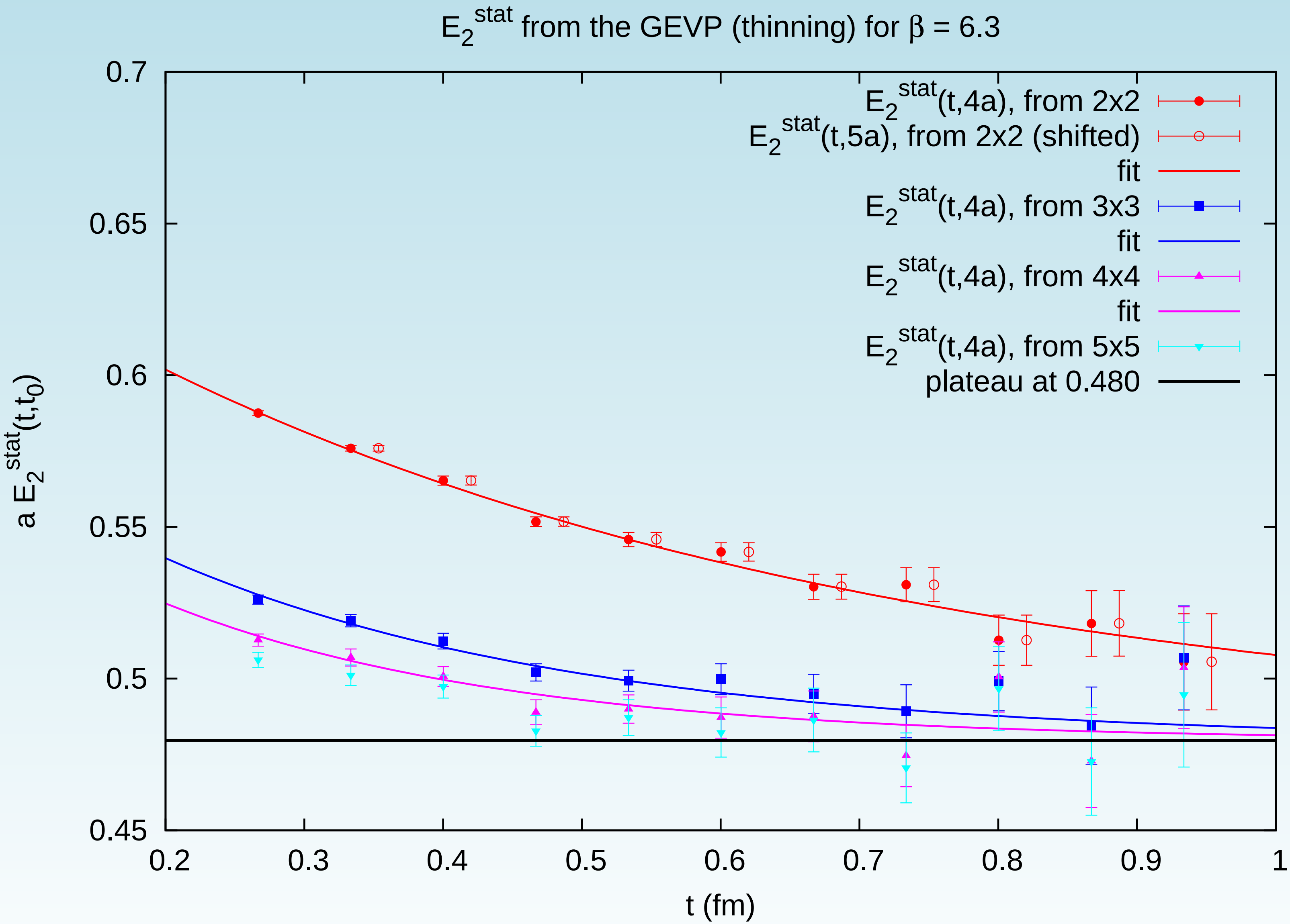
Spectrum: (Static) Excited State, 1st basis



Spectrum: Static Energy, 2nd basis

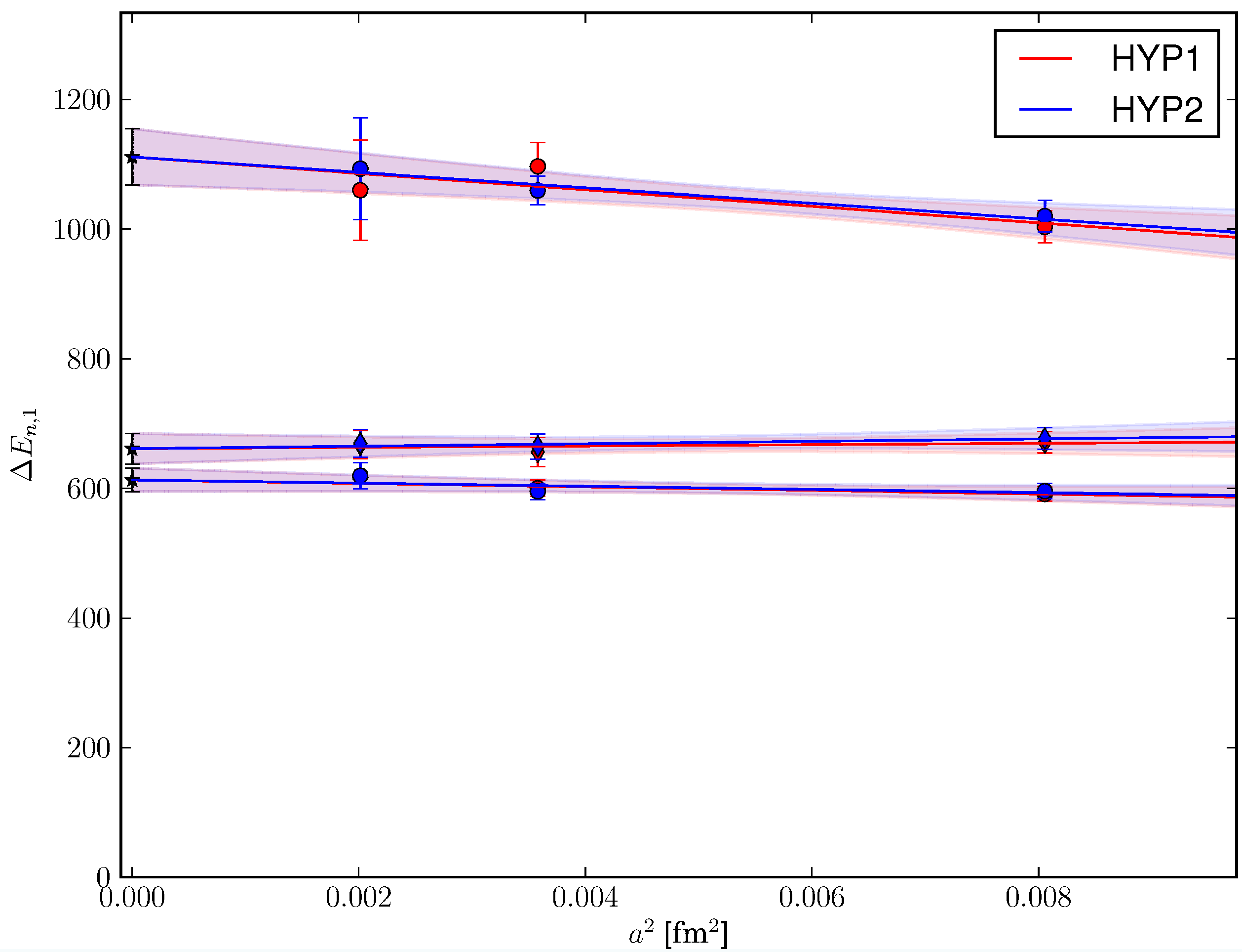


Spectrum: (Static) Excited State, 2nd basis



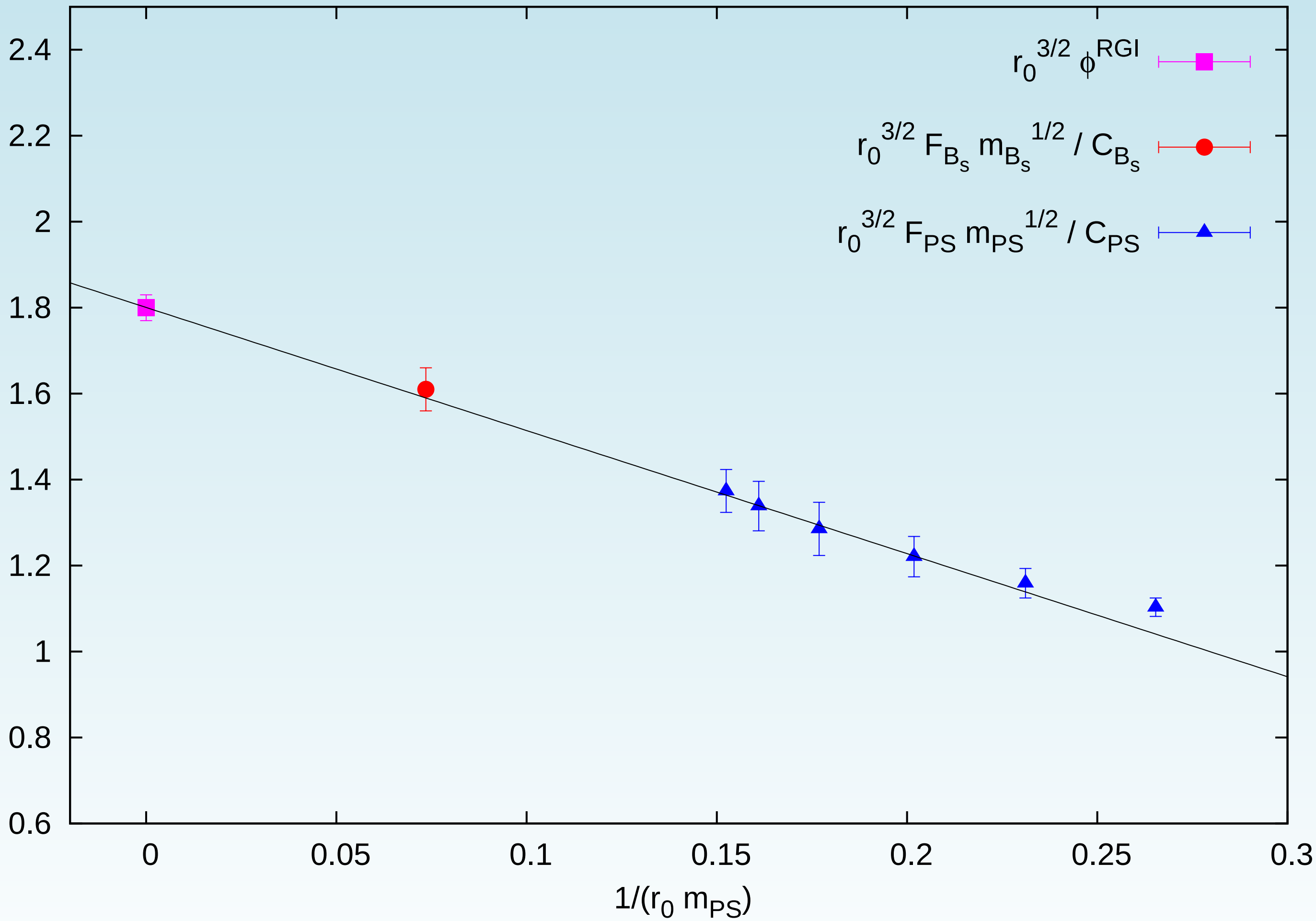
Continuum Limit (I): Spectrum

Energy splittings (in MeV): ΔE_{21} (static and total) and ΔE_{31}



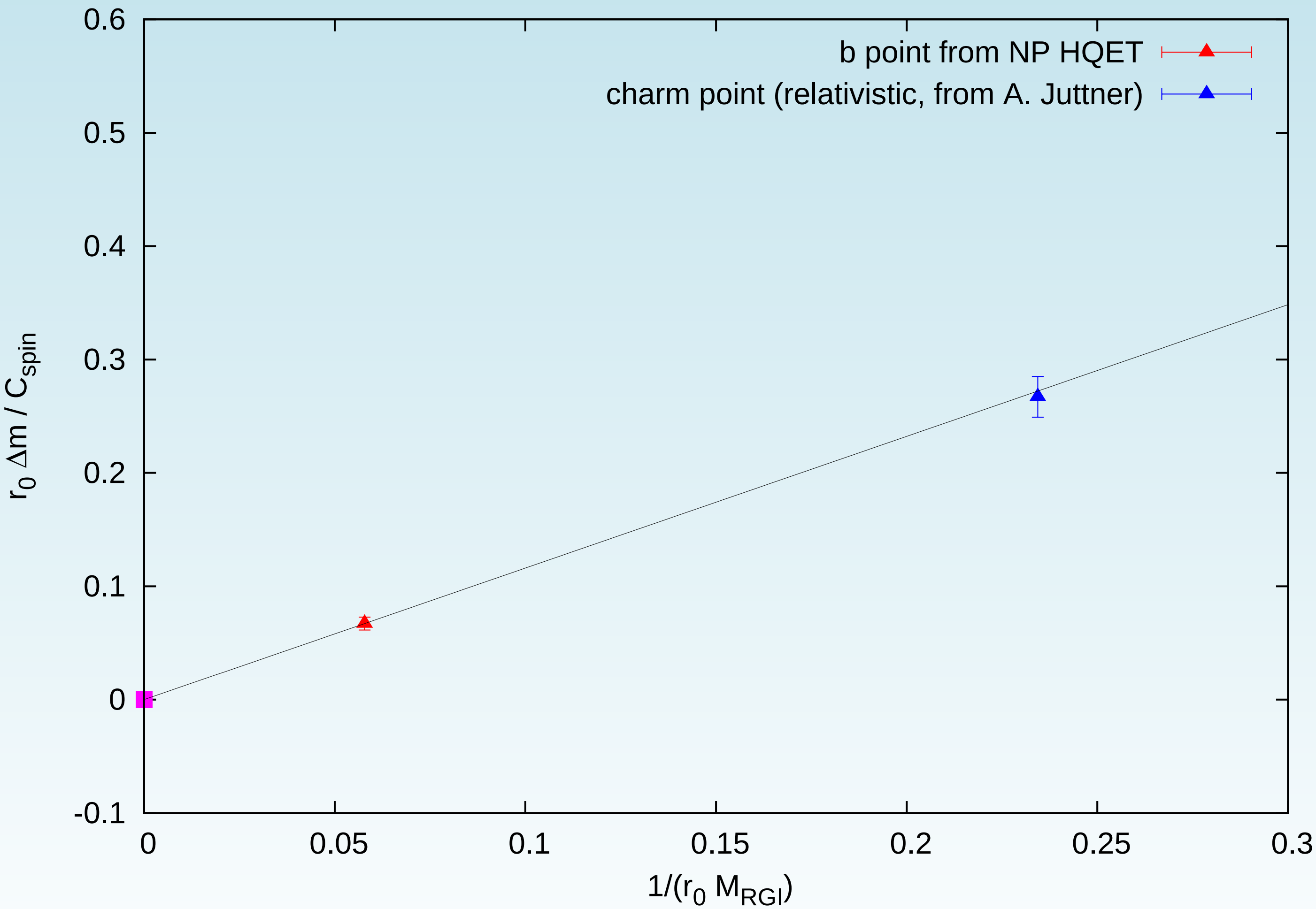
Comparison with Charm Region

PS meson decay constant: static (magenta) and b (red) points plus LQCD data from Della Morte et al., JHEP 2008 (blue points)



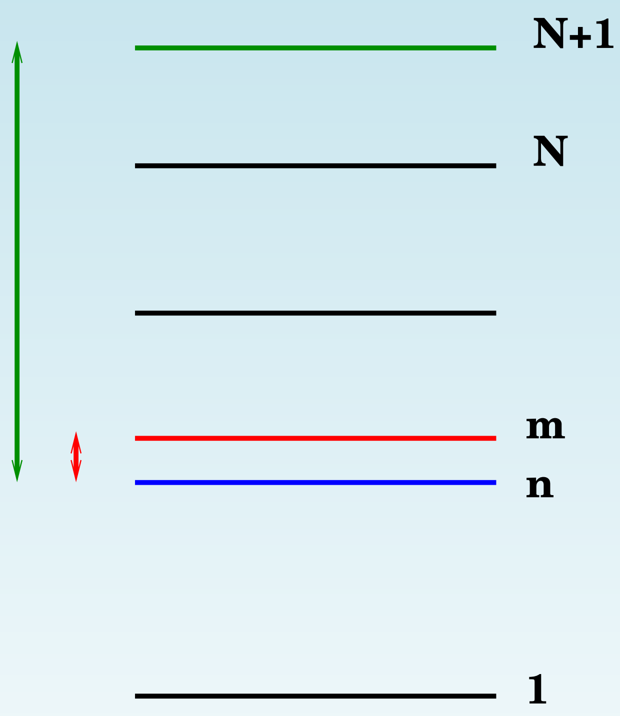
Spin Splitting - Preliminary

Comparison of mass difference $B_s^* - B_s$ for static (magenta), b (red) and charm (blue) points



Conclusions (I)

Efficient GEVP



- GEVP studied analytically, using perturbation theory to get corrections to truncated $N \times N$ problem, taking large t and t_0.
- For $t \leq 2t_0$, leading corrections suppressed by the large energy gap $E_{N+1} - E_n$.
- Corrections are understood, expected form helps in fits of the data.
- Nothing beats a good plateau!

Conclusions (II)

Fully NP heavy-light (B_s) mesons (quenched) to order $1/m$

- A NP result needs a NP computation (renormalization)
- NP-determined HQET parameters in action and currents are precise enough for 1) few % precision in matrix elements and 2) few MeV precision in energy levels
- a^{-n} divergences are no serious problem
- Ground-state (bare) matrix elements are also precise enough when GEVP is used efficiently (note: 100 configs)
- HQET $+\ 1/m$ corrections agrees well with interpolation between static point and charm region (linearity in $1/m$ extends to the charm point!)