

# HANDLING EXCITED STATES ON THE LATTICE: THE GEVP METHOD\*

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High-precision calculations of hadron spectroscopy are a crucial task for lattice QCD. State-of-the-art techniques are needed to disentangle the contributions from different energy states, such as solving the generalized eigenvalue problem (GEVP) for zero-momentum hadron correlators in an efficient way. We review the method and discuss its application in the determination of the  $B_s$ -meson spectrum using (quenched) nonperturbative HQET at the order of  $1/m_b$ .

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## 1. Introduction

Systematic errors in lattice simulations include not only finite-size and discretization effects, dependence on the chiral extrapolation and quenching, but also systematic effects due to contamination from higher excited states in the calculation of energy levels (masses) of quark bound states. This is because masses and decay constants are computed in lattice QCD from the exponential decay of Euclidean correlation functions  $C(t)$ , which are built from composite fields with the quantum numbers of a given state (see *e.g.* [1]). More precisely, in the simulation, one evolves gluon fields (the link variables  $U$ ) in the Monte Carlo dynamics associated with the partition function

$$Z = \int \mathcal{D}U e^{-S_g} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\int d^4x \bar{\psi}(x) K \psi(x)} = \int \mathcal{D}U e^{-S_g} \det K(U), \quad (1)$$

where  $S_g$  is the gluonic action and  $K(U)$  is the Dirac operator. (The quenched approximation corresponds to  $\det K = 1$ .) Although the quark fields  $\psi$  are not evolved directly, information about them may be obtained

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once the link configuration is produced, since quark propagators are given by  $\langle \psi \bar{\psi} \rangle = \langle K^{-1} \rangle$ , *i.e.* by computing the inverse of  $K(U)$  for each configuration of the link variables and averaging over the configurations produced. Similarly, the computed inverse of  $K(U)$  may be used to build interpolators, *i.e.* products of creation and annihilation operators with the quantum numbers of the desired bound state and a good overlap with the hadron wave function on the lattice. The result is then averaged over the configurations to yield the (Euclidean) correlators  $C(t)$  as

$$C(t) = \sum_{\mathbf{x}} \langle J(\mathbf{x}, t) J(0, 0) \rangle \equiv \langle O(t) O(0) \rangle, \quad (2)$$

where  $J(\mathbf{x}, t) = \bar{\psi} \Gamma \psi$  and  $\Gamma$  is the appropriate Dirac matrix (*e.g.*  $\Gamma = \gamma_5$  for pseudoscalar mesons). Finally, one determines masses and decay constants by identifying the various contributions to the spectral decomposition

$$\langle O(t) O(0) \rangle = C(t) = \sum_{n=1}^{\infty} |\langle n | \hat{O} | 0 \rangle|^2 e^{-E_n t}, \quad (3)$$

where  $|n\rangle$  are eigenstates of the Hamiltonian (*i.e.* the logarithm of the transfer matrix) and all energies  $E_n$  have the vacuum energy subtracted. Also, we assume Hermitian operators and a large enough time extent of the lattice to yield the simple exponential form above. At large  $t$  we expect to observe a plateau in the “effective mass”

$$E_1^{\text{eff}}(t) \equiv \log[C(t)/C(t+1)] \rightarrow E_1 + \mathcal{O}\left(e^{-(E_2-E_1)t}\right), \quad (4)$$

in such a way that the true ground-state energy  $E_1$  may be estimated.

Clearly, determining masses and decay constants from the correlators in Eq. (3) is not an easy task. To see this, consider the first correction above, given by  $\exp[-(E_2 - E_1)t]$  with a positive coefficient, in the case of a heavy-light system. For typical energy differences of a few hundred MeV, a plateau can only be reached for  $t$  around 1 fm, but by then the signal has started to compete with noise, even for improved static-quark discretizations. This is a general problem and trying to determine subleading corrections by multiple-exponential fits leads to large systematic errors. One alternative is to use more sophisticated fitting methods, such as Bayesian fitting, evolutionary fitting and NMR-inspired methods. Another way to ensure better precision is inspired by the variational method in quantum mechanics and consists in increasing the basis of interpolators to build a matrix of correlators  $C_{ij}(t)$ , for which a Generalized Eigenvalue Problem (GEVP) is formulated (see *e.g.* [2]). One then considers all-to-all propagators [3] instead of simple point sources as indicated in Eq. (2).

The GEVP is a valuable tool to reduce systematic errors in the above determinations, and thus to deliver high-precision tests of QCD. We summarize the derivation of an optimal use of the method in Section 2 below and describe its application to spectrum calculations of  $B_s$  mesons in non-perturbative HQET to order  $1/m_b$  in Section 3.

### 2. The method

The GEVP is defined by

$$C(t) v_n(t, t_0) = \lambda_n(t, t_0) C(t_0) v_n(t, t_0), \tag{5}$$

where  $t > t_0$  and  $C(t)$  is now a matrix of correlators, given by

$$C_{ij}(t) = \langle O_i(t) O_j(0) \rangle = \sum_{n=1}^{\infty} e^{-E_n t} \Psi_{ni} \Psi_{nj}, \quad i, j = 1, \dots, N. \tag{6}$$

The chosen interpolators  $O_i$  are taken (hopefully) linearly independent, *e.g.* they may be built from smeared quark fields using  $N$  different smearing levels. The matrix elements  $\Psi_{ni}$  are defined by

$$\Psi_{ni} \equiv (\Psi_n)_i = \langle n | \hat{O}_i | 0 \rangle, \quad \langle m | n \rangle = \delta_{mn}. \tag{7}$$

One thus computes  $C_{ij}$  for the interpolator basis  $O_i$  from the numerical simulation, then gets effective energy levels  $E_n^{\text{eff}}$  and estimates for the matrix elements  $\Psi_{ni}$  from the solution  $\lambda_n(t, t_0)$  of the GEVP at large  $t$ . For the energies

$$E_n^{\text{eff}}(t, t_0) \equiv \frac{1}{a} \log \frac{\lambda_n(t, t_0)}{\lambda_n(t+a, t_0)} \tag{8}$$

it is shown [2] that  $E_n^{\text{eff}}(t, t_0)$  converges exponentially as  $t \rightarrow \infty$  (and fixed  $t_0$ ) to the true energy  $E_n$ . However, since the exponential falloff of higher contributions may be slow, it is also essential to study the convergence as a function of  $t_0$  in order to achieve the required efficiency for the method. This has been done in [4], by explicit application of (ordinary) perturbation theory to a hypothetical truncated problem where only  $N$  levels contribute. The solution in this case is exactly given by the true energies, and corrections due to the higher states are treated perturbatively. We get

$$E_n^{\text{eff}}(t, t_0) = E_n + \varepsilon_n(t, t_0) \tag{9}$$

for the energies and

$$e^{-\hat{H}t} \left( \hat{Q}_n^{\text{eff}}(t, t_0) \right)^\dagger |0\rangle = |n\rangle + \sum_{n'=1}^{\infty} \pi_{nn'}(t, t_0) |n'\rangle \tag{10}$$

for the eigenstates of the Hamiltonian, which may be estimated through

$$\hat{Q}_n^{\text{eff}}(t, t_0) = R_n(\hat{O}, v_n(t, t_0)), \tag{11}$$

$$R_n = (v_n(t, t_0), C(t) v_n(t, t_0))^{-1/2} \left[ \frac{\lambda_n(t_0 + a, t_0)}{\lambda_n(t_0 + 2a, t_0)} \right]^{t/2}. \tag{12}$$

In our analysis we see that, due to cancellations of  $t$ -independent terms in the effective energy, the first-order corrections in  $\varepsilon_n(t, t_0)$  are independent of  $t_0$  and very strongly suppressed at large  $t$ . We identify two regimes: (1) for  $t_0 < t/2$ , the 2nd-order corrections dominate and their exponential suppression is given by the smallest energy gap  $|E_m - E_n| \equiv \Delta E_{m,n}$  between level  $n$  and its neighboring levels  $m$ ; and (2) for  $t_0 \geq t/2$ , the first-order corrections dominate and the suppression is given by the large gap  $\Delta E_{N+1,n}$ . Amplitudes  $\pi_{nn'}(t, t_0)$  get main contributions from the first-order corrections. For fixed  $t - t_0$  these are also suppressed with  $\Delta E_{N+1,n}$ . Clearly, the appearance of large energy gaps in the second regime improves convergence significantly. A pictorial illustration of the improvement is shown in Fig. 1. We therefore work with  $t, t_0$  combinations in this regime.

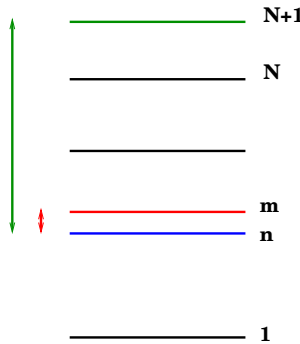


Fig.1. Schematic representation of energy levels, showing how a solution of the GEVP for conveniently chosen  $t, t_0$  yields conversion to the asymptotic state controlled by a much larger energy gap than usual (*i.e.* the one represented by the longer arrow instead of the shorter one).

A very important step of our approach is to realize that the same perturbative analysis may be applied to get the leading corrections to correlators in an effective theory, such as corrections of order  $1/m_b$  to the static case in HQET correlation functions. These are given by

$$C_{ij}(t) = C_{ij}^{\text{stat}}(t) + \omega C_{ij}^{1/m_b}(t) + \mathcal{O}(\omega^2), \tag{13}$$

where the combined  $\mathcal{O}(1/m_b)$  corrections are symbolized by the expansion parameter  $\omega$ . Following the same procedure as above, we get similar expo-

nential suppressions (with the static energy gaps) for static and  $\mathcal{O}(1/m_b)$  terms in the effective theory. We arrive at

$$E_n^{\text{eff}}(t, t_0) = E_n^{\text{eff,stat}}(t, t_0) + \omega E_n^{\text{eff},1/m_b}(t, t_0) + \mathcal{O}(\omega^2) \quad (14)$$

with

$$E_n^{\text{eff,stat}}(t, t_0) = E_n^{\text{stat}} + \beta_n^{\text{stat}} e^{-\Delta E_{N+1,n}^{\text{stat}} t} + \dots, \quad (15)$$

$$E_n^{\text{eff},1/m_b}(t, t_0) = E_n^{1/m_b} + \left[ \beta_n^{1/m_b} - \beta_n^{\text{stat}} t \Delta E_{N+1,n}^{1/m_b} \right] e^{-\Delta E_{N+1,n}^{\text{stat}} t} + \dots \quad (16)$$

and similarly for matrix elements.

An application of the methods described in this section is discussed next.

### 3. Application to nonperturbative HQET

High-precision hadronic matrix elements are a key ingredient as theoretical inputs in  $B$  physics and are ideally obtained from lattice-QCD simulations. However, currently used lattices are not large enough to represent simultaneously the low-energy scale of  $\Lambda_{\text{QCD}}$ , which requires a large physical lattice size, and the high-energy scale of the heavy-quark mass  $m_b$ , which requires a very small lattice spacing  $a$ . A promising alternative is to consider (lattice) heavy-quark effective theory (HQET), which allows for an elegant theoretical treatment, with the possibility of fully nonperturbative renormalization [5].

HQET provides a valid low-momentum description for systems with one heavy quark, with manifest heavy-quark symmetry in the static limit. The heavy-quark flavor and spin symmetries are broken at finite values of  $m_b$  respectively by kinetic and spin terms, with first-order [*i.e.*  $\mathcal{O}(1/m_b)$ ] corrections to the static Lagrangian incorporated by an expansion of the statistical weight in  $1/m_b$ , such that the symmetry-breaking operators are treated as insertions into static correlation functions. This guarantees the existence of a continuum limit, with results that are independent of the regularization, provided that the renormalization be done nonperturbatively. Masses and decay constants are expanded as sums of a static and an  $\mathcal{O}(1/m_b)$  contribution, in terms of the parameters of the effective theory and of the bare energies and matrix elements, which are computed in the numerical simulation. The divergences (with inverse powers of  $a$ ) in these parameters are cancelled through the nonperturbative renormalization, which is based on matching the HQET parameters to QCD on lattices of small physical volume — where fine lattice spacings can be considered — and extrapolating to a large volume by the step-scaling method. This analysis has been recently

completed for the quenched case [6]. Using the computed HQET parameters, we have carried out a study [7] (see also [8]) of spectrum and decay constants for  $B_s$  mesons applying the GEVP method as described in the previous section.

We have employed two lattice actions for the static quark, lattices of spatial extent  $L \approx 1.5$  fm with three lattice spacings and all-to-all strange-quark propagators constructed from approximate low modes, with 100 configurations. The interpolating fields were obtained from a simple  $\gamma_0\gamma_5$  structure and 8 levels of Gaussian smearing for the strange-quark field. The resulting  $(8 \times 8)$  correlation matrix may be conveniently truncated to an  $N \times N$  one and the GEVP solved for each  $N$ , so that results can be studied as a function of  $N$ . We have used two methods for picking a basis from the above interpolators and checked that both yielded the same results.

The combined use of nonperturbatively determined HQET parameters and efficient GEVP solution allowed us to reach a precision of a few percent in matrix elements and of a few MeV in energy levels, even with only a moderate number of configurations. A corresponding study for the  $N_f = 2$  case is in progress.

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