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Efficient use of the Generalized Eigenvalue Problem

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We analyze the systematic errors made when using the generalized eigenvalue problem to extract energies and matrix elements in lattice gauge theory. Effective theories such as HQET are also discussed. Numerical results are shown for the extraction of ground-state and excited B-meson masses and the ground-state decay constant in the static approximation.

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1. The Generalized Eigenvalue Problem

1.1 History

At a conference in 1981, K. Wilson suggested to use a variational technique to compute energy levels in lattice gauge theory [1]. The idea was picked up and applied to the glueball spectrum [2,3] and to the static quark potential(s) [4]. With a certain choice of the variational basis $\{\phi_i\,, i=1\ldots N\}$ and maximizing $\langle\phi|\mathrm{e}^{-(t-t_0)\hat{H}}|\phi\rangle/\langle\phi|\phi\rangle$ with $|\phi\rangle=\sum_i\alpha_i|\phi_i\rangle$, the variational technique yields the generalized eigenvalue problem (GEVP). It is applicable beyond the computation of the ground-state energy and has been widely used, but rarely in the form where it can be shown that corrections to the true energy levels decrease exponentially for large time [5].

Apart from [5], statements about corrections due to higher energy levels seem to be absent in the literature. We here add such statements and suggest a somewhat different use of the GEVP, which we will show to be more efficient under certain conditions. We also treat the case of an effective theory and show numerical results for heavy-quark effective theory (HQET).

1.2 Basic idea

We start from a matrix of correlation functions on an infinite-time lattice

$$C_{ij}(t) \;=\; \langle O_i(0)O_j(t)\rangle = \sum_{n=1}^{\infty}\mathrm{e}^{-E_nt}\,\psi_{ni}\psi_{nj}\,,\quad i,j=1,\ldots,N \tag{1.1}$$
$$\psi_{ni}\equiv(\psi_n)_i=\langle n|\hat{O}_i|0\rangle\quad E_n\le E_{n+1}\,.$$

For simplicity we assume real ψ_{ni}. States $|n\rangle$ with $\langle m|n\rangle=\delta_{mn}$ are eigenstates of the transfer matrix and all energies have the vacuum energy subtracted. $O_j(t)$ are any gauge-invariant fields on a timeslice t that correspond to Hilbert-space operators $\hat{O}_j$ whose quantum numbers are then also carried by the states $|n\rangle$. Besides the energy levels E_n one may want to determine a matrix element

$$p_{0n}=\langle 0|\hat{P}|n\rangle \tag{1.2}$$

of an operator $\hat{P}$ that may or may not be in the set of operators $\left\{\hat{O}_i\right\}$. Starting from the GEVP,

$$C(t)\,v_n(t,t_0)=\lambda_n(t,t_0)\,C(t_0)\,v_n(t,t_0)\,,\quad n=1,\ldots,N\quad t>t_0, \tag{1.3}$$

Lüscher and Wolff showed that [5]

$$E_n=\lim_{t\to\infty}E_n^{\rm eff}(t,t_0)\,,\quad E_n^{\rm eff}(t,t_0)=\frac{1}{a}\log\frac{\lambda_n(t,t_0)}{\lambda_n(t+a,t_0)}\,. \tag{1.4}$$

For a while we now assume that only N states contribute,

$$C_{ij}(t)=C_{ij}^{(0)}(t)=\sum_{n=1}^{N}\mathrm{e}^{-E_nt}\,\psi_{ni}\psi_{nj}\,. \tag{1.5}$$

We introduce the dual (time-independent) vectors u_n, defined by $(u_n,\psi_m)=\delta_{mn}\,,\ m,n\le N$, with $(u_n,\psi_m)\equiv\sum_{i=1}^{N}(u_n)_i\,\psi_{mi}$. Inserting into eq. (1.5) gives

$$C^{(0)}(t)u_n=\mathrm{e}^{-E_nt}\,\psi_n\,,\quad C^{(0)}(t)\,u_n=\lambda_n^{(0)}(t,t_0)\,C^{(0)}(t_0)\,u_n\,. \tag{1.6}$$

So the GEVP is solved by

$$\lambda_n^{(0)}(t,t_0) = \mathrm{e}^{-E_n(t-t_0)}\,, \quad v_n(t,t_0) \propto u_n \tag{1.7}$$

and there is an orthogonality for all t of the form

$$(u_m, C^{(0)}(t)\, u_n) = \delta_{mn}\, \rho_n(t)\,, \quad \rho_n(t) = \mathrm{e}^{-E_n t}\,. \tag{1.8}$$

These equations mean that the operators $\hat{Q}_n = \sum_{i=1}^N (u_n)_i \hat{O}_i \equiv (\hat{O}, u_n)$ create the eigenstates $|n\rangle = \hat{Q}_n|0\rangle$ of the Hamilton operator: $\hat{H}|n\rangle = E_n\,|n\rangle$. Consequently we have $p_{0n} = \langle 0|\hat{P}|n\rangle = \langle 0|\hat{P}\hat{Q}_n|0\rangle$, which, preparing for a generalization, we may rewrite as

$$p_{0n} = \sum_{j=1}^N \langle P(t) O_j(0)\rangle (u_n)_j = \frac{\sum_{j=1}^N \langle P(t) O_j(0)\rangle\, v_n(t,t_0)_j}{(v_n(t,t_0)\,, C(t)\, v_n(t,t_0))^{1/2}} \frac{\lambda_n(t_0+t/2,t_0)}{\lambda_n(t_0+t,t_0)}\,, \tag{1.9}$$

while for all t, t_0 we have $E_n^{\mathrm{eff}}(t,t_0) = E_n$.

Let us now come back to the general case eq. (1.1). The idea is to solve the GEVP, eq. (1.3), "at large time" where the contribution of states $n > N$ is small and obtain matrix elements and energy levels from

$$E_n^{\mathrm{eff}} = \frac{1}{a} \log \frac{\lambda_n(t,t_0)}{\lambda_n(t+a,t_0)} = E_n + \varepsilon_n(t,t_0) \tag{1.10}$$

$$p_{0n}^{\mathrm{eff}} = \frac{\sum_{j=1}^N \langle P(t_1) O_j(0)\rangle\, (v_n(t,t_0))_j}{(v_n(t,t_0)\,, C(t_2)\, v_n(t,t_0))^{1/2}} \frac{\lambda_n(t_0+t_2/2,t_0)}{\lambda_n(t_0+t_1,t_0)} = p_{0n} + \pi_n(t,t_0) \quad \text{at } t_1 = t_2 = t\,. \tag{1.11}$$

The restriction to $t_1 = t_2 = t$ is for simplicity. The corrections ε_n, π_n will disappear at large times. Note that in the literature the energy levels are often not extracted in this way. Rather, the standard effective masses of correlators made from $Q_n = (O, v_n(t,t_0))$ are used, and the question of the size of the corrections is left open. However, the form in eq. (1.10) has a theoretical advantage as it was shown in [5] that (at fixed t_0)

$$\varepsilon_n(t,t_0) = \mathrm{O}(\mathrm{e}^{-\Delta E_n t})\,, \quad \Delta E_n = \min_{m \neq n} |E_m - E_n|\,. \tag{1.12}$$

This is non-trivial as it allows to obtain the excited levels with corrections that vanish in the limit of large t, keeping t_0 fixed. However, it appears from this formula that the corrections can be very large when there is an energy level close to the desired one. This is the case in interesting phenomena such as string breaking [6,7], where in numerical applications the corrections appeared to be very small despite the formula above[1]. Also in static-light systems the gaps are typically only around $\Delta E_n \approx 400\,\mathrm{MeV}$, and in full QCD with light quarks a small gap $\Delta E_n \approx 2m_\pi$ appears in some channels.

Our contribution to the issue is a more complete discussion of the correction ε_n to E_n as well as a discussion of the corrections π_n to the matrix elements. It turns out that a very useful case is to consider the situation

$$t \leq 2t_0\,, \tag{1.13}$$

[1] In fact a different formula was claimed in [6].

e.g. with $t - t_0 = $ const. or $2 \geq t/t_0 = $ const., and then take t_0 (in practice moderately) large. Then it is not difficult to show that

$$\varepsilon_n(t,t_0) \;=\; \mathrm{O}(\mathrm{e}^{-\Delta E_{N+1,n}\, t})\,, \quad \Delta E_{m,n} = E_m - E_n\,, \tag{1.14}$$

$$\pi_n(t,t_0) \;=\; \mathrm{O}(\mathrm{e}^{-\Delta E_{N+1,n}\, t_0})\,, \quad \text{at fixed } t - t_0 \tag{1.15}$$

$$\pi_1(t,t_0) \;=\; \mathrm{O}(\mathrm{e}^{-\Delta E_{N+1,1}\, t_0}\mathrm{e}^{-\Delta E_{2,1}\,(t-t_0)}) + \mathrm{O}(\mathrm{e}^{-\Delta E_{N+1,1}\, t})\,. \tag{1.16}$$

The large gaps $\Delta E_{N+1,n}$ can solve the problem of close-by levels for example in the string-breaking situation, but also speed up the general convergence very much. For example in static-light systems $\Delta E_{6,1} \approx 2\,\mathrm{GeV}$ means that roughly a factor of 5 in time separation is gained. We now turn to an outline of the proof of these statements.

2. Perturbation theory

We start from the solutions above for $C = C^{(0)}$ and treat the higher states as perturbations. This perturbative evaluation was already set up by F. Niedermayer and P. Weisz a while ago [8] but never published. We noted the advantage of $t \leq 2t_0$, the form of the corrections to the effective matrix elements defined above and could show that these relations hold to all orders in the expansion.

We want to obtain λ_n and v_n in a perturbation theory in ε, where

$$Av_n = \lambda_n B v_n\,, \quad A = A^{(0)} + \varepsilon A^{(1)}\,, \quad B = B^{(0)} + \varepsilon B^{(1)}\,. \tag{2.1}$$

We will set

$$A^{(0)} \;=\; C^{(0)}(t)\,, \quad \varepsilon A^{(1)} = C^{(1)}(t)\,, \tag{2.2}$$

$$B^{(0)} \;=\; C^{(0)}(t_0)\,, \quad \varepsilon B^{(1)} = C^{(1)}(t_0) \tag{2.3}$$

in the end. The solutions of the lowest-order equation $A^{(0)} v_n^{(0)} \;=\; \lambda_n^{(0)} B^{(0)}\, v_n^{(0)}$ satisfy an orthogonality relation $(v_n^{(0)}, B^{(0)} v_m^{(0)}) = \rho_n\, \delta_{nm}$ as in eq. (1.8) above. Writing

$$\lambda_n \;=\; \lambda_n^{(0)} + \varepsilon\lambda_n^{(1)} + \varepsilon^2\lambda_n^{(2)}\,\ldots\,, \quad v_n \;=\; v_n^{(0)} + \varepsilon v_n^{(1)} + \varepsilon^2 v_n^{(2)}\,\ldots \tag{2.4}$$

we get for the first two orders

$$A^{(0)} v_n^{(1)} + A^{(1)} v_n^{(0)} \;=\; \lambda_n^{(0)}\,\left[B^{(0)} v_n^{(1)} + B^{(1)} v_n^{(0)}\right] + \lambda_n^{(1)}\, B^{(0)} v_n^{(0)}\,, \tag{2.5}$$

$$A^{(0)} v_n^{(2)} + A^{(1)} v_n^{(1)} \;=\; \lambda_n^{(0)}\,\left[B^{(0)} v_n^{(2)} + B^{(1)} v_n^{(1)}\right] + \lambda_n^{(1)}\,\left[B^{(0)} v_n^{(1)} + B^{(1)} v_n^{(0)}\right] + \lambda_n^{(2)}\, B^{(0)} v_n^{(0)}\,. \tag{2.6}$$

With the orthogonality of the lowest-order vectors, $v_n^{(0)}$, one obtains just like in ordinary QM perturbation theory the solutions for eigenvalues and eigenvectors

$$\lambda_n^{(1)} \;=\; \rho_n^{-1}\left(v_n^{(0)}, \Delta_n v_n^{(0)}\right)\,, \quad \Delta_n \equiv A^{(1)} - \lambda_n^{(0)} B^{(1)} \tag{2.7}$$

$$v_n^{(1)} \;=\; \sum_{m \neq n} \alpha_{nm}^{(1)}\, \rho_m^{-1/2}\, v_m^{(0)}\,, \quad \alpha_{nm}^{(1)} = \rho_m^{-1/2}\,\frac{\left(v_m^{(0)}, \Delta_n v_n^{(0)}\right)}{\lambda_n^{(0)} - \lambda_m^{(0)}} \tag{2.8}$$

$$\lambda_n^{(2)} \;=\; \sum_{m \neq n} \rho_n^{-1}\rho_m^{-1}\,\frac{\left(v_m^{(0)}, \Delta_n v_n^{(0)}\right)^2}{\lambda_n^{(0)} - \lambda_m^{(0)}} - \rho_n^{-2}\left(v_n^{(0)}, \Delta_n v_n^{(0)}\right)\left(v_n^{(0)}, B^{(1)} v_n^{(0)}\right)\,. \tag{2.9}$$

Also a recursion formula can be given for the higher-order coefficients.

2.1 Application to the perturbations $C^{(1)}$

Now we insert our specific problem eq. (2.2), eq. (2.3). With straightforward algebra and with a representation (for $m > n$)

$$(\lambda_n^{(0)} - \lambda_m^{(0)})^{-1} \,=\, (\lambda_n^{(0)})^{-1}(1-\mathrm{e}^{-(E_m-E_n)(t-t_0)})^{-1} \,=\, (\lambda_n^{(0)})^{-1}\sum_{k=0}^{\infty}\mathrm{e}^{-k(E_m-E_n)(t-t_0)}\,, \quad (2.10)$$

one finds the correction terms listed at the end of the first section. Initially this is so for the first two orders, but the mentioned recursions allow to show that the higher orders are even more suppressed.

2.2 Effective theory to first order

In an effective theory, all correlation functions

$$C_{ij}(t) \,=\, C_{ij}^{\mathrm{stat}}(t) + \omega C_{ij}^{1/\mathrm{m}}(t) + \mathrm{O}(\omega^2) \quad (2.11)$$

are computed in an expansion in a small parameter, ω, which we consider to first order only. The notation is taken from HQET where $\omega \propto 1/m$.

We start from the GEVP in the full theory, eq. (1.3), and use the form of the correction terms of the effective energies ($t \leq 2t_0$)

$$E_n^{\mathrm{eff}}(t,t_0) \,=\, \log\frac{\lambda_n(t,t_0)}{\lambda_n(t+a,t_0)} \,=\, E_n + \mathrm{O}(\mathrm{e}^{-\Delta E_{N+1,n}t}), \quad (2.12)$$

see the discussion above. Expanding this equation in ω, we have

$$E_n^{\mathrm{eff,stat}}(t,t_0) \,=\, a^{-1}\log\frac{\lambda_n^{\mathrm{stat}}(t,t_0)}{\lambda_n^{\mathrm{stat}}(t+a,t_0)} \,=\, E_n^{\mathrm{stat}} + \mathrm{O}(\mathrm{e}^{-\Delta E_{N+1,n}^{\mathrm{stat}}t})\,, \quad (2.13)$$

$$E_n^{\mathrm{eff,1/m}}(t,t_0) \,=\, \frac{\lambda_n^{1/\mathrm{m}}(t,t_0)}{\lambda_n^{\mathrm{stat}}(t,t_0)} - \frac{\lambda_n^{1/\mathrm{m}}(t+a,t_0)}{\lambda_n^{\mathrm{stat}}(t+a,t_0)} \,=\, E_n^{1/\mathrm{m}} + \mathrm{O}(t\,\mathrm{e}^{-\Delta E_{N+1,n}^{\mathrm{stat}}t})\,. \quad (2.14)$$

Here $\mathrm{O}(t\,\mathrm{e}^{-Et})$ is a summary for terms $(b_0+b_1t)\mathrm{e}^{-Et}$. As expected for first-order perturbation theory, only the eigenvectors of the static GEVP

$$C^{\mathrm{stat}}(t)\,v_n^{\mathrm{stat}}(t,t_0) \,=\, \lambda_n^{\mathrm{stat}}(t,t_0)\,C^{\mathrm{stat}}(t_0)\,v_n^{\mathrm{stat}}(t,t_0)\,, \quad (2.15)$$

with normalization $(v_m^{\mathrm{stat}}(t,t_0)\,, C^{\mathrm{stat}}(t_0)\,v_n^{\mathrm{stat}}(t,t_0)) = \delta_{mn}$, are needed in the formula

$$\lambda_n^{1/\mathrm{m}}(t,t_0) \,=\, \left(v_n^{\mathrm{stat}}(t,t_0)\,, [C^{1/\mathrm{m}}(t) - \lambda_n^{\mathrm{stat}}(t,t_0)C^{1/\mathrm{m}}(t_0)]v_n^{\mathrm{stat}}(t,t_0)\right) \quad (2.16)$$

for the first-order corrections in ω.

Similarly one may expand

$$p_{01}^{\mathrm{eff}} \,=\, p_{01}^{\mathrm{eff,stat}} + \omega\, p_{01}^{\mathrm{eff,1/m}} + \mathrm{O}(\omega^2)$$

$$p_{01}^{\mathrm{eff,1/m}} \,=\, p_{01}^{1/\mathrm{m}} + \mathrm{O}[\mathrm{e}^{-\Delta E_{N+1,1}^{\mathrm{stat}}t_0}\,\mathrm{e}^{-\Delta E_{2,1}^{\mathrm{stat}}(t-t_0)}\,(\Delta E_{N+1,1}^{1/\mathrm{m}}t_0 + \Delta E_{2,1}^{1/\mathrm{m}}(t-t_0))] \quad (2.17)$$

and an explicit expression for $p_{01}^{\mathrm{eff,1/m}}$ is easily given. Again it involves only the solutions of the lowest-order (in ω) GEVP, v_n^{stat} and $\lambda_n^{\mathrm{stat}}$, together with the first-order correlators $C^{1/\mathrm{m}}$. The large energy gap $\Delta E_{N+1,1}$ controls the corrections.

3. Application to static-light B_s-mesons

We have carried out a test in quenched HQET, discretizing the static quark by the HYP2 action and the strange quark by the non-perturbatively $O(a)$-improved Wilson action. Space-time is $2L \times L^3$ with periodic boundary conditions, $L \approx 1.5\,\mathrm{fm}$ and we consider two lattice spacings: $0.1\,\mathrm{fm}$ and $0.07\,\mathrm{fm}$ ($\beta = 6.0219$ and 6.2885), respectively with $\kappa = 0.133849\,,\ 0.1349798$. The all-to-all strange-quark propagators [9] are constructed from 50 (approximate) low modes and two noise fields on each timeslice of 100 configurations.

The gauge links entering in the interpolating fields are smeared with 3 iterations of (spatial) APE smearing [10,11]. Then 8 different levels of Gaussian smearing [12] are applied to the strange-quark field and we use a simple $\gamma_0\gamma_5$ structure in Dirac space for all 8 interpolating fields. The local field (no smearing) is included to compute the decay constant. The resulting 8×8 correlation function is first truncated to an $N \times N$ one projecting with the N eigenvectors of $C(t_i)$ with the largest eigenvalues. Here t_i is taken to be roughly 0.2 fm (i.e. $t_i = 2a$ at $\beta = 6.0219$ and $3a$ at $\beta = 6.2885$). With N not too large, this avoids numerical instabilities and large statistical errors in the GEVP [13]. We present our results for the spectrum and for the decay constant below.

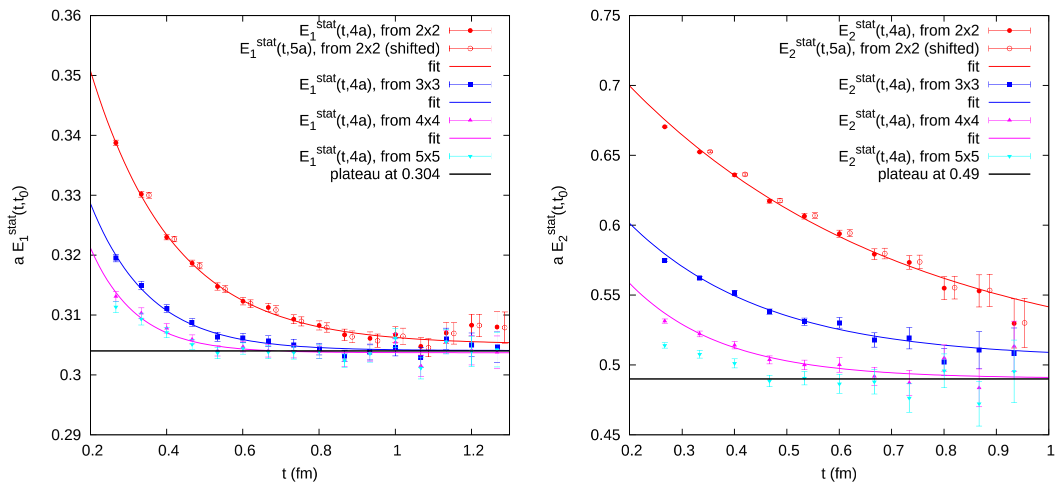

Figure 1: *The estimate* $aE_n^{\mathrm{eff,stat}}(t,t_0)$*,* $n = 1,2$*, as a function of* t*, for* $N = 2,3,4,5$ *from top to bottom at* $a = 0.07\,\mathrm{fm}$*. The curves are* $E_n + \alpha_N\,\mathrm{e}^{-\Delta E_{N+1,1}\,t}$ *(see comment about* $\Delta E_{N+1,1}$ *in the text). The coefficients* α_N *are fitted for each* N*.*

Figure 1 shows the effective energies eq. (1.10) for the lowest two levels at $a = 0.07\,\mathrm{fm}$. Statistical errors for the ground-state effective energy are below a level of about $3\,\mathrm{MeV}$ for time separations $t \leq 1\,\mathrm{fm}$. Unexpectedly, these errors are roughly independent of t_0 and of $N \leq 5$. The functional form of the systematic corrections eq. (1.14) works very well down to surprisingly small t and the independence of t_0 is confirmed by the data. Since the corrections are well understood to be below the MeV–level for $t > 0.6\,\mathrm{fm}\,, N \geq 4$, we may quote for example E_1^{stat} with a total error of about $1\,\mathrm{MeV}$. We emphasize that what counts is of course the time separation in physical units. The data at the coarser lattice spacing are very similar.

For this analysis, the energy gaps on the coarser lattice, $a\Delta E_{N+1,1} \approx 0.46, 0.65, 0.83$, respectively for $N = 2,3,4$, have been taken from plateaux of $aE_n^{\mathrm{eff,stat}}(t,t_0)$ for $N = 6$. They have then been appropriately rescaled with the lattice spacing. A similar procedure has been used for $a\Delta E_{N+1,2}$.

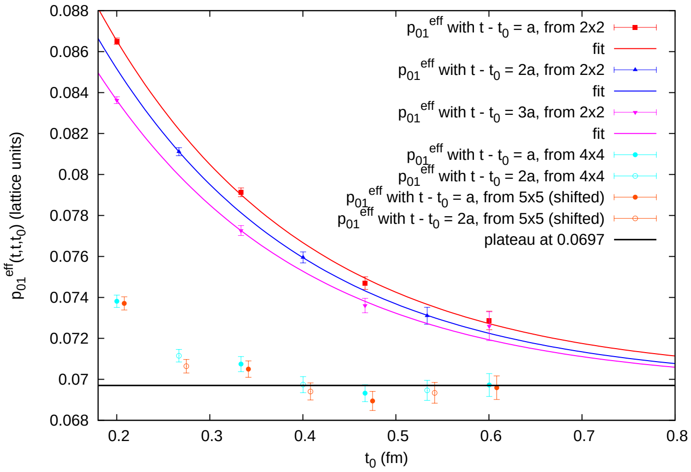

Figure 2: *Bare effective static decay constant as a function of t_0 for different values of $t-t_0$ at $a = 0.07\,\mathrm{fm}$. The curves are $F + \alpha_N\,\mathrm{e}^{-\Delta E_{N+1,1}t_0}$ (see comment about $\Delta E_{N+1,1}$ in the text).*

Figure 2 shows the effective decay constant, eq. (1.14), at the smaller lattice spacing. The leading corrections again dominate at small time already. For $N = 5$ there is a rather early plateau around $t_0 = 0.4\,\mathrm{fm}$, where both excited-state corrections are well below the % level and the statistical errors are around $0.7\,\%$. The same statements hold for $a = 0.10\,\mathrm{fm}$. Note that we fit the corrections separately for each $t-t_0$ and N as a function of t_0. The decay of the fit parameters α_N as a function of $t-t_0$ is of the expected form eq. (1.16).

4. Conclusions

From a detailed analysis of the corrections to the eigen–values and vectors of the GEVP, it becomes clear that t_0 should not be made too small. In particular if $t_0 \geq t/2$, the simple forms eq. (1.14), eq. (1.15) can be shown. These corrections decay exponentially with the large gaps $E_{N+1} - E_n$. For first-order corrections in an effective theory a similar suppression holds, with the energy differences of the lowest-order theory.

As pointed out to us at the conference, the authors of [14] studied the GEVP for a toy model with ten states and noted that it is relevant to have t_0 “large enough”. Fig.17 of [14] indeed illustrates that the effective energies become independent of t_0 when (roughly) $t_0 \geq t/2$ is respected.

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