

## The Shifman-Vainshtein-Zakharov method: Why it works, why it fails, and ways to improve it

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Shifman, Vainshtein, and Zakharov (SVZ) have proposed a procedure for calculating hadronic masses and determining nonperturbative parameters in QCD using the operator-product expansion for two-point functions and (exponential) moments of the corresponding spectral functions. In this paper we present a detailed theoretical analysis of the SVZ procedure in the context of nonrelativistic potential theory. We find that the *phenomenological* success of the usual first-order SVZ method in relating hadronic energies (masses) is due to a hidden variational principle and a semiclassical structure which gives correct JWKB-type relations between energies. The *first-order* method fails *theoretically*: it does not reproduce the correct potential-model or field-theoretic parameters, e.g., the gluon-condensate parameter of QCD. We show why it breaks down in this application, and that its reliability can be greatly improved in all applications by using higher-order approximations for the moment function. Our results are directly relevant for the SVZ analysis of charmonium and  $b$ -quarkonium. The general conclusions should also hold for light-quark systems.

### I. INTRODUCTION

In a series of papers published in 1979, Shifman, Vainshtein, and Zakharov<sup>1</sup> (SVZ) showed that one could use the dispersion relations for two-point functions in QCD in combination with first-order perturbation theory and the operator-product expansion to determine the masses of quark-antiquark bound states in terms of parameters in the field theory. The SVZ procedure has now been used to correlate masses and spin splittings of a large number of  $q\bar{q}$  states in terms of a few parameters.<sup>1-3</sup> For example, if it is applied to charmonium, with the QCD parameters adjusted to fit the  $J/\psi$  mass, the predictions for the  $^1S_0$ ,  $^1P_1$ , and  $^3P_{0,1,2}$  masses agree with the observed masses to within a few tens of MeV.<sup>2,3</sup>

This success has been remarkable, but mysterious. Bell and Bertlmann<sup>4,5</sup> studied the nonrelativistic SVZ procedure numerically using potential models in an attempt to assess its reliability. They found that the usual first-order method failed to give accurate energies for known potentials, and conversely, failed to reproduce the potential parameters from given energies. As an example, the analog of the gluon-condensate parameter was underestimated by a factor of 2.

In this paper, we show in the context of nonrelativistic potential models for the  $q\bar{q}$  system that the success of the first-order SVZ procedure in correlating energies, and its failure in predicting absolute energies or determining parameters, are consequences of the structure of the approximation scheme. This structure includes a hidden variational principle for the ground-state energy  $E_{1S}$  and a hidden semiclassical approximation which gives JWKB-type relations among the energies  $E_{1l}$  for different angular momenta  $l$  and different quark masses.

In one class of phenomenological applications of the SVZ procedure, the potential parameters—or QCD condensate parameters—are adjusted to fit  $E_{1S}$ , for example, in charmonium. The semiclassical structure in the first-order approximation then guarantees that the nearby energies  $E_{1l}$  are given with reasonable accuracy, and that the predictions for  $b$ -quarkonium are also valid. This success in simultaneously fitting many energies does not imply that the first-order SVZ procedure is reliable in other applications. It is not. The variational principle for  $E_{1S}$  shows, in fact, that the analog of the gluon-condensate parameter in the operator-product expansion is necessarily underestimated by a large amount in the fits to charmonium, a fact already noted empirically by Bell and Bertlmann.<sup>4,5</sup> We conclude that the field-theoretic parameters obtained using SVZ are suspect.

To see if it is possible to eliminate these problems, we extend the nonrelativistic SVZ analysis to higher order and obtain substantial improvement. We show that we can further improve the results for singular interactions by making a Padé-type resummation of the perturbation series. Our results suggest strongly that it would be worthwhile to extend the field-theoretic calculations to include nonleading terms in the operator-product expansion.

We also show by counterexample that it is not possible to determine the form of the  $q\bar{q}$  confining interaction using the finite-order SVZ method or its nonrelativistic limit.<sup>6</sup> This has the unfortunate consequence that information about  $q\bar{q}$  excited states which is easily obtained in potential models is not accessible from the present low-order SVZ method.

The organization of the paper is as follows: In Secs. IIA and IIB, we review the SVZ program and set up its nonrelativistic analog. In Sec. IIC we develop criteria for

determining the bound-state energies from the SVZ exponential moment function  $R(\tau)$ . In Sec. IID, we prove a variational bound on  $E_{1S}$  in terms of the first-order approximation to  $R(\tau)$ . In Secs. IIE and IIF we generalize our results to arbitrary angular momentum and derive our semiclassical relation for  $E_{1l}$ .

In Sec. IIIA we test our results for general power-law potentials including the realistic Coulomb-plus-linear potential, and show that the first-order SVZ technique "works" only when the potential parameters are adjusted to fit the lowest-energy levels (a particularly striking example for charmonium and  $b$ -quarkonium is given in Table II). We extend our results to second (and higher) orders in the perturbation series for  $R(\tau)$  in Sec. IIIB and show that substantial improvements result. Padé summation of the series is considered in Sec. IIIC, and the problems in determining the interaction by the SVZ technique are discussed in Sec. IIID. Finally, we summarize our results and discuss their implications for the SVZ program in Sec. IIIE.

## II. THEORETICAL ANALYSIS

### A. Background

The Shifman-Vainshtein-Zakharov (SVZ) program is an extension of the old idea of duality,<sup>7</sup> e.g., for the process  $e^+e^- \rightarrow$  hadrons, in which the average behavior of the observed, highly structured cross section is described using low-order QCD results for the "free" cross section for  $e^+e^- \rightarrow q\bar{q}$ .<sup>7-9</sup> Duality has been used to test perturbative QCD,<sup>8,10</sup> determine quark masses and predict leptonic widths for vector-meson decays,<sup>7,11</sup> and to estimate gluonic radiative corrections to these widths.<sup>12</sup> It was realized by SVZ (Ref. 1) that one could go further by including some nonperturbative effects in the theoretical calculations, and use duality to predict the masses of  $q\bar{q}$  bound states.

To implement their program for  $e^+e^-$  annihilation via a virtual photon, SVZ used the duality relations obtained by repeated differentiation of the dispersion relation satisfied by the photon vacuum-polarization function  $\Pi(q^2)$ ,

$$\frac{1}{N!} \left[ -\frac{d}{dQ^2} \right]^N \Pi(-Q^2) = \frac{1}{\pi} \int dW^2 \frac{\text{Im}\Pi(W^2)}{(W^2+Q^2)^{N+1}}, \quad Q^2 = -q^2. \quad (1)$$

$\text{Im}\Pi(s)$  is related to the physical cross section for  $e^+e^- \rightarrow \gamma \rightarrow$  hadrons at the center-of-mass energy  $W$  by

$$\text{Im}\Pi(W^2) = \frac{W^2\sigma(W)}{16\pi^2\alpha^2e_q^2}, \quad (2)$$

where we restrict our attention to a single- (heavy-) quark flavor. The right-hand side of Eq. (1) is therefore just an energy average of  $W^2\sigma$  calculated by convoluting  $W^2\sigma$  with a smearing function  $f(W^2+Q^2) \propto (W^2+Q^2)^{-N-1}$ , and reduces for a sum of narrow resonances ( $q\bar{q}$  bound states) and a continuum to

$$\begin{aligned} & \frac{1}{\pi} \int dW^2 \frac{\text{Im}\Pi(W^2)}{(W^2+Q^2)^{N+1}} \\ &= \frac{3}{4\pi} \sum_n \frac{M_n\Gamma_n(e^+e^-)}{(M_n^2+Q^2)^{N+1}} \\ &+ \frac{1}{16\pi^3\alpha^2e_q^2} \int_{s_0}^{\infty} dW^2 \frac{W^2\sigma(W)}{(W^2+Q^2)^{N+1}}, \end{aligned} \quad (3)$$

where  $M_n$  and  $\Gamma_n(e^+e^-)$  are the mass and leptonic width of the  $n$ th resonance.

The left-hand side of Eq. (1) can be calculated by using perturbative QCD and the operator-product expansion to evaluate the vacuum expectation value of the time-ordered product of quark currents

$$i \int d^4x e^{iq \cdot x} \langle 0 | T(j_\mu(x), j_\nu(0)) | 0 \rangle = (q_\mu q_\nu - q^2 g_{\mu\nu}) \Pi(q^2), \quad (4)$$

and is given to first order in  $\alpha_s$  by

$$\begin{aligned} & \frac{1}{N!} \left[ -\frac{d}{dQ^2} \right]^N \Pi(-Q^2) \\ &= A_N(Q^2) [1 + \alpha_s a_N(Q^2) + (\phi_1/16m_q^4) b_N(Q^2)]. \end{aligned} \quad (5)$$

The functions  $A_N$ ,  $a_N$ , and  $b_N$  were calculated for  $Q^2=0$  by SVZ,<sup>1</sup> and for general  $Q^2$  by Reinders, Rubenstein, and Yazaki (RRY).<sup>2</sup> The constant  $\phi_1$  is the nonperturbative gluon-condensate parameter which appears in the leading correction in the operator-product expansion,

$$\phi_1 = \frac{4\pi\alpha_s}{9} \langle 0 | G_{\mu\nu}^a G_a^{\mu\nu} | 0 \rangle, \quad (6)$$

where  $G$  is the gluon field-strength tensor.

For  $N$  sufficiently large, only the ground state of the  $q\bar{q}$  system contributes significantly to the sum in Eq. (3), and Eqs. (1), (3), and (5) give a relation connecting the mass  $M_1$  and leptonic width  $\Gamma_1(e^+e^-)$  of the  $q\bar{q}$  ground state to the field-theoretic expression. The ratio of Eqs. (1) for two successive values of  $N$  is independent of  $\Gamma_1(e^+e^-)$  and depends linearly on  $M_1^2$ . By requiring that this ratio be stationary with respect to variations in  $N$  (and  $Q^2$ ), SVZ (Ref. 1) and RRY (Ref. 2) could determine  $\phi_1$  in terms of the  $J/\psi$  mass  $M_1$  (we note that  $\alpha_s$  and  $m_q$  were determined using moments with  $N$  small), and could then use the result with sum rules for different two-point functions to predict the masses of other states, e.g., the  $^1S_0$ ,  $^3P_0$ ,  $^3P_1$ ,  $^3P_2$ , and  $^1P_1$  states in charmonium.

In later work, SVZ replaced the inverse power moments of  $W^2\sigma$  with respect to  $(W^2+Q^2)$  defined by Eq. (3) by "exponential moments" which further emphasize the contribution of the ground state to the sum rule and make it easier to determine the ground-state energy. The exponential moments are obtained by applying a Borel transform to Eq. (1). This involves multiplying Eq. (1) by  $(Q^2)^{N+1}$  and taking the limit  $N \rightarrow \infty$  with the ratio  $\lambda = N/Q^2$  fixed. The right-hand sides of Eqs. (1) and (3) are then replaced by an exponentially weighted average of the physical cross section,

$$\begin{aligned}
M(\lambda) &= \frac{1}{\pi} \int dW^2 e^{-\lambda W^2} \text{Im}\Pi(W^2) \\
&= \frac{3}{4\pi} \sum_n M_n \Gamma_n (e^+ e^-) e^{-\lambda M_n^2} \\
&\quad + \frac{1}{16\pi^3 \alpha^2 e_q^2} \int_{s_0}^{\infty} dW^2 W^2 \sigma(W) e^{-\lambda W^2}, \quad (7)
\end{aligned}$$

while the left-hand side of Eq. (1) is replaced by the Borel transform of Eq. (5) (explicit results are given by Bertlmann<sup>3</sup>).

It is clear from Eq. (7) that the exact value of the function  $R(\lambda) = -d \ln M(\lambda) / d\lambda$  approaches  $M_1^2$  as  $\lambda \rightarrow \infty$ . While the approximate QCD expression for  $M(\lambda)$  is not reliable for  $\lambda$  large, SVZ suggest that one can nevertheless obtain a good value of  $M_1^2$  by evaluating  $R_{\text{approx}}$  at a point where this function is stable with respect to variations of  $\lambda$ ,  $dR_{\text{approx}}/d\lambda = 0$ . (This corresponds in the power-moments method to evaluating the ratio of successive moments in the region of stability with respect to  $N$ .) The advantages of the exponential-moments method have been discussed by SVZ,<sup>1</sup> Bell and Bertlmann,<sup>4,5</sup> and Vainshtein *et al.*<sup>13</sup> We will use exponential moments in the following analysis of the SVZ program.

#### B. The SVZ program for potential models

To study the reasons for the unexpected success of the SVZ program, we will model the  $q\bar{q}$  system using nonrelativistic potential models in which the quarks are confined in a Schrödinger potential  $V(r)$ , and attempt to determine the ground-state energy  $E_{1l}$  for angular momentum  $l$  using a first-order (or low-order) perturbation expansion of the appropriate two-point function and the SVZ exponential moments. The first-order  $S$ -wave problem was studied for simple power-law potentials by Bell and Bertlmann<sup>4,5</sup> who showed that the SVZ procedure gave reasonably good results for  $E_{1S}$ , but did not provide an explanation for that success. Those authors also showed that the exponential-moments method was generally more accurate than the power-moments method used in most of the work of SVZ (Ref. 1) and RRY.<sup>2</sup> Bertlmann<sup>3</sup> later used the nonrelativistic exponential-moment limit of the RRY power moments to study  $P$ -wave energies in the charm ( $\psi$ ) and bottom ( $\Upsilon$ ) systems, and found that the nonrelativistic and relativistic results agreed to  $\sim 10$  MeV for these heavy-quark systems.

In the following sections, we will repeat the Bell-Bertlmann<sup>4,5</sup> analysis of the nonrelativistic  $S$ -wave problem and show *why* the SVZ procedure works in this case. We will then extend the first-order analysis to general  $l$ , again with emphasis on the reasons for its success. Finally in Sec. III, we will give a number of numerical examples, and show how the results are improved by going to higher order in the perturbation expansion.

The nonrelativistic photon vacuum-polarization function is simply a multiple of the  $q\bar{q}$  energy Green's function evaluated at the origin,

$$\Pi(E) \rightarrow \frac{2}{3} m_q^2 \tilde{G}(0,0,E), \quad (8)$$

where

$$\tilde{G}(\vec{r}', \vec{r}, E) = \int_{-\infty}^{\infty} dt e^{iEt} G(\vec{r}', \vec{r}, t) \quad (9)$$

and

$$G(\vec{r}', \vec{r}, t) = i\theta(t) K(\vec{r}', \vec{r}, t). \quad (10)$$

Here  $K(\vec{r}', \vec{r}, t)$  is the Feynman propagation function which describes the propagation of an initial  $q\bar{q}$  state forward ( $t > 0$ ) or backward ( $t < 0$ ) in time, and is given explicitly by the usual sum over states,

$$K(\vec{r}', \vec{r}, t) = \sum_{nlm} \psi_{nlm}(\vec{r}') e^{-iE_{nlm}t} \psi_{nlm}^*(\vec{r}), \quad (11)$$

where  $\psi_{nlm}(\vec{r})$  is the  $q\bar{q}$  wave function for principal quantum number  $n$ , orbital angular momentum  $l$ , and magnetic quantum number  $m$ . (We will suppress the spin quantum numbers which are irrelevant in the following arguments.) The cross section  $W^2 \sigma_{\text{bound}}$  for  $e^+ e^- \rightarrow (q\bar{q} \text{ bound state})$  is proportional to  $\tilde{K}(0,0,E)$  (Refs. 14 and 15) and depends only on the  $S$  states,

$$W^2 \sigma_{\text{bound}}(E) = 12\pi^2 \alpha^2 e_q^2 m_q^{-2} \tilde{K}(0,0,E), \quad (12)$$

where

$$\begin{aligned}
\tilde{K}(0,0,E) &= \int_{-\infty}^{\infty} dt e^{iEt} K(0,0,t) \\
&= 2\pi \sum_{n=1}^{\infty} |\psi_{nS}(0)|^2 \delta(E - E_{nS}). \quad (13)
\end{aligned}$$

The Green's function  $\tilde{G}(0,0,E)$  satisfies a dispersion relation which follows from Eqs. (9)–(13):

$$\tilde{G}(0,0,E) = \frac{1}{\pi} \int_0^{\infty} dE' \frac{\text{Im}\tilde{G}(0,0,E')}{E' - E}, \quad (14)$$

where

$$\begin{aligned}
\text{Im}\tilde{G}(0,0,E) &= \frac{1}{2} \tilde{K}(0,0,E) \\
&= \pi \sum_{n=1}^{\infty} |\psi_{nS}(0)|^2 \delta(E - E_{nS}). \quad (15)
\end{aligned}$$

The dispersion relations analogous to the SVZ relations in Eq. (3) are obtained by repeated differentiation of Eq. (14),

$$\begin{aligned}
\frac{1}{N!} \left[ \frac{d}{dE} \right]^N \tilde{G}(0,0,E) &= \frac{1}{\pi} \int_0^{\infty} dE' \frac{\text{Im}\tilde{G}(0,0,E')}{(E' - E)^{N+1}} \\
&= \frac{m_q^2}{24\pi^3 \alpha^2 e_q^2} \int_0^{\infty} dE' \frac{W^2 \sigma_{\text{bound}}(E')}{(E' - E)^{N+1}}. \quad (16)
\end{aligned}$$

Application of the Borel transform<sup>1,13</sup>

$$\hat{B} = \lim_{\substack{N \rightarrow \infty \\ E = -N/\tau}} (-E)^{N+1} (\cdot) \quad (17)$$

to Eq. (16) gives the nonrelativistic version of the exponential SVZ moments defined in Eq. (7),

$$\begin{aligned}
\hat{B} \left[ \frac{2\pi}{N!} \left[ \frac{d}{dE} \right]^N \tilde{G}(0,0,E) \right] \\
&= \frac{m_q^2}{12\pi^2 \alpha^2 e_q^2} \int_0^{\infty} dE' e^{-E'\tau} W^2 \sigma_{\text{bound}}(E') \\
&= \sum_{n=1}^{\infty} |\psi_{nS}(0)|^2 e^{-E_{nS}\tau}. \quad (18)
\end{aligned}$$

The sum in Eq. (18) is just the Euclidean or imaginary time form of the Feynman propagation function for  $\vec{r}' = \vec{r} = 0$ ,

$$K(0,0,-i\tau) = \sum_n |\psi_{nS}(0)|^2 e^{-E_{nS}\tau}. \quad (19)$$

We may therefore identify the left-hand side of Eq. (18) with  $K(0,0,-i\tau)$  and rewrite Eq. (18) in a form similar to the relativistic expression in Eq. (7),

$$K(0,0,-i\tau) = \frac{m_q^2}{12\pi^2\alpha^2 e_q^2} \int_0^\infty dE e^{-E\tau} W^2 \sigma_{\text{bound}}(E). \quad (20)$$

Equation (20) is a special case of the general duality relation for  $e^+e^-$  annihilation studied in the preceding paper<sup>16</sup> (we will denote this paper by WDD).

The ground-state energy  $E_{1S}$  of the  $q\bar{q}$  system can clearly be calculated from Eq. (19) or (20) as

$$E_{1S} = \lim_{\tau \rightarrow \infty} R_0(\tau), \quad (21)$$

where

$$R_0(\tau) = -\frac{d}{d\tau} \ln K(0,0,-i\tau), \quad l=0, \quad (22)$$

provided the large- $\tau$  behavior of  $R_0(\tau)$  is known. The SVZ procedure (already studied by Bell and Bertlmann<sup>4</sup> for power-law potentials) uses instead the expression for  $R_0(\tau)$  obtained in first-order perturbation theory, and estimates  $E_{1S}$  as

$$E_{1S} \approx R_0^{(1)}(\tau_{\min}), \quad (23)$$

where  $\tau_{\min}$  is the value of  $\tau$  for which  $dR^{(1)}/d\tau = 0$ . It is by no means clear on the surface that this procedure should work: The perturbation expansion is essentially a small- $\tau$  expansion [see the discussion in WDD (Ref. 16)], yet one is trying to determine the large- $\tau$  behavior of  $K(0,0,-i\tau)$ . The "magic"<sup>4</sup> in the procedure is that it works reasonably well, as shown in Table I. To show *why*, we will first study the general properties of the limiting procedure in Eq. (21), and will then show that Eq. (23) gives what is essentially a Rayleigh-Ritz variational estimate for  $E_{1S}$ .

TABLE I. Comparison of the exact ground-state energies for the power-law potentials  $V(r) = V_0 r^\nu$  given in Ref. 4, Table I, with the results obtained using the first-order perturbative expansion of  $R(\tau)$  and the SVZ procedure [ $E_{1S}^{(1)} = \min_\tau R^{(1)}(\tau)$ ] and its variational improvement ( $E_{1S,\text{var}} = \min_\tau [R^{(1)}(\tau) - 1/4\tau]$ ). The energies are given in units of  $V_0^{2/(2+\nu)} m_q^{-\nu/(2+\nu)}$ .

$\nu$	$E_{1S}$ exact	$E_{1S}^{(1)}$	$E_{1S}$ variational
-1	$-\frac{1}{4}$	-0.131	-0.157
$-\frac{1}{2}$	-0.438	-0.369	-0.392
$\frac{1}{2}$	1.833	1.977	1.906
1	2.338	2.616	2.461
2	3	3.464	3.162
4	3.800	4.500	3.985

### C. Properties of $R_0(\tau)$ and the determination of $E_{1S}$

If we follow SVZ (Ref. 1) and Bell and Bertlmann<sup>4,5</sup> and attempt to determine  $E_{1S}$  from a low-order perturbation expansion of  $R_0(\tau)$  (first order in the cases considered by those authors), the approximate  $R_0(\tau)$  will not have the proper asymptotic behavior for  $\tau \rightarrow \infty$ , and the limiting procedure in Eq. (21) will fail. We therefore need a criterion for selecting a "best" value for our approximate  $E_{1S}$ . We can easily establish two useful criteria from formal properties of  $R_0(\tau)$ . It is convenient for this purpose to introduce a discrete normalized, positive distribution function  $\{f\} = \{f_n, n=1,2,\dots\}$ , with the functions  $f_n$  defined by

$$f_n(\tau) = |\psi_{nS}(0)|^2 e^{-E_{nS}\tau} / \sum_{n=1}^{\infty} |\psi_{nS}(0)|^2 e^{-E_{nS}\tau}. \quad (24)$$

$R_0(\tau)$  is then given by

$$R_0(\tau) = \langle E \rangle_\tau = E_{1S} + \langle E - E_{1S} \rangle_\tau \geq E_{1S}, \quad (25)$$

where the average  $\langle \cdot \rangle_\tau$  is calculated with respect to  $\{f\}$ . The final inequality follows from the ordering of the energy eigenvalues and the positivity of  $\{f\}$ , and establishes the (obvious) fact that  $R_0(\tau)$  approaches its limit from above. A simple calculation shows in addition that

$$\begin{aligned} dR_0/d\tau &= -\langle E^2 \rangle + \langle E \rangle^2 \\ &= -\langle (E - \langle E \rangle)^2 \rangle < 0. \end{aligned} \quad (26)$$

The approach of  $R_0(\tau)$  to its limit is therefore monotonic. The difference  $(R - E_{1S})$  is of order  $e^{-(E_{2S} - E_{1S})\tau}$  for  $\tau \rightarrow \infty$ .

Bell and Bertlmann<sup>4,5</sup> observed that (for all the potentials they considered) the first-order approximation to  $R_0$  always has a minimum as a function of  $\tau$ , and took this minimum for their best estimate of the ground-state energy

$$E_{1S}^{(1)} \approx \min_\tau [R_0^{(1)}(\tau)]. \quad (27)$$

This choice was of course motivated by the fact that the exact  $R_0(\tau)$  must approach its limit (monotonically) from above. [The same is true for the ratios  $R_l(\tau)$  defined for arbitrary orbital angular momentum  $l$  in Sec. II E.] We will show in the next section that it corresponds also to a variational calculation of  $E_{1S}$  and that  $E_{1S}^{(1)} > E_{1S}$ .

Unfortunately, the minimum in the approximate  $R_0$  can disappear in higher orders of perturbation theory. We therefore consider the next derivative,

$$d^2 R_0/d\tau^2 = \langle (E - \langle E \rangle)^3 \rangle. \quad (28)$$

This quantity does not have a definite sign for an arbitrary distribution function. However, for the specific distribution defined by Eq. (24), we can show that  $d^2 R/d\tau^2 > 0$  for  $\tau$  not too large,  $(E_{2S} - E_{1S})\tau \lesssim 1$ , by using the relation<sup>17</sup> (valid in the JWKB approximation)

$$|\psi_{nS}(0)|^2 = \frac{m_q^{3/2}}{4\pi^2} \sqrt{E_n} \frac{dE_n}{dn} \quad (29)$$

and replacing sums by integrals. For  $\tau$  large,  $f_1 \gg f_2 \gg \dots$ , a direct calculation neglecting terms of

order  $f_n^2$  for  $n > 1$  also gives  $d^2R_0/d\tau^2 > 0$ . The latter condition holds in the regions with which we will be mostly concerned. We conclude that a change in sign of  $d^2R_0/d\tau^2$  as  $\tau$  increases signals a departure from the expected behavior, and will use the value of  $\tau$  at the inflection point in  $R_0(\tau)$  to calculate the approximate value of  $E_{1S}$ . This procedure is remarkably successful, as will be shown in Sec. III.

The minimum and inflection-point criteria for determining optimum estimates for the energy can also be used to determine  $E_{1l}$ , the ground-state energy for angular momentum  $l$ , from the ratios  $R_l(\tau)$  defined in Sec. II E. The derivations are similar to that given here.

We remark finally that neither of the criteria above *guarantees* the existence of a bound state unless the approximate  $E_{1S}$  is negative. They simply provide ways to determine a best estimate for  $E_{1S}$  if it is *assumed* that a bound state exists. The same assumption is implicit in all applications of the relativistic SVZ procedure.

#### D. The variational principle

Bell and Bertlmann<sup>4,5</sup> noted that  $R^{(1)}(\tau)$  always has a minimum for power-law potentials, and that the minimum value  $E_{1S}^{(1)}$  was always greater than the exact ground-state

$$E_{1S} \leq \int d^3r \phi^* H \phi / \int d^3r \phi^* \phi = \int d^3r \phi^* \left[ -\frac{\nabla^2}{m_q} + V(r) \right] \phi / \int d^3r \phi^* \phi \quad (32)$$

for any normalizable trial wave function  $\phi(r)$ . The second term in Eq. (31) is exactly equal to the potential term in Eq. (32) for the trial function

$$\phi(r) = r^{1/2} e^{-mr^2/2\tau}. \quad (33)$$

We therefore use this trial function in Eq. (32) and find after calculating the kinetic energy term that for any  $\tau > 0$

$$\begin{aligned} E_{1S} &\leq \frac{5}{4\tau} + \frac{m_q^2}{2\pi\tau^2} \int d^3r e^{-m_q r^2/\tau} r V(r) \\ &= R_0^{(1)} - \frac{1}{4\tau} < R_0^{(1)}. \end{aligned} \quad (34)$$

Thus,  $E_{1S}$  is *strictly less* than the approximate value determined by the minimum of  $R_0^{(1)}(\tau)$ ,<sup>20</sup>

$$E_{1S} < E_{1S}^{(1)} = \min_{\tau} [R_0^{(1)}(\tau)]. \quad (35)$$

The value of  $E_{1S}$  obtained by minimizing  $(R_0^{(1)} - 1/4\tau)$  instead of  $R_0^{(1)}$  is always somewhat better than  $E_{1S}^{(1)}$ , but as shown in Table I, the improvement is not spectacular for simple power-law potentials [the correction term  $1/4\tau$  is generally small near the minimum of  $R_0^{(1)}(\tau)$ ]. Much better trial wave functions are easily found, e.g., a simple Gaussian without the factor  $r^{1/2}$  which appears in Eq. (33). However, our intent is to test the SVZ procedure, and we do not know of a relativistic version of the Rayleigh-Ritz variational principle which is applicable to their problem. We will therefore drop the variational approach.

The existence of the hidden variational principle<sup>21</sup> has two important implications. First, it explains why the SVZ procedure gives a reasonable estimate for  $E_{1S}$  (Table

energy  $E_{1S}$ :  $E_{1S}^{(1)} > E_{1S}$ . We will show next that this inequality holds for general potentials as a consequence of the Rayleigh-Ritz variational principle. This (hidden) variational principle makes the best possible use of the limited input in the first-order SVZ procedure, and accounts, we believe, for its (theoretically unexpected) success.

The Euclidean propagator  $K(0,0,-i\tau)$  is given to first order for a general potential  $V(r)$  by<sup>18</sup>

$$\begin{aligned} K(0,0,-i\tau) &= \left[ \frac{m_q}{4\pi\tau} \right]^{3/2} \\ &\times \left[ 1 - \frac{m_q}{2\pi} \int d^3r \frac{e^{-m_q r^2/\tau}}{r} V(r) + \dots \right]. \end{aligned} \quad (30)$$

Expanding  $-\ln K$  to first order in  $V$  (Ref. 19) and calculating its derivative with respect to  $\tau$ , we find that

$$R_0^{(1)} = \frac{3}{2\tau} + \frac{m_q^2}{2\pi\tau^2} \int d^3r r e^{-m_q r^2/\tau} V(r). \quad (31)$$

The Rayleigh-Ritz variational principle states that

I and Sec. III A) even though the values of  $\tau$  which minimize  $R_0^{(1)}(\tau)$  are so large that the first-order expansion is invalid:  $\tau$  is used only as a Rayleigh-Ritz variational parameter in Eq. (27). Second,  $E_{1S}^{(1)}$  is the best estimate for  $E_{1S}$  which can be obtained using the first-order procedure. We can only improve the approximation to  $E_{1S}$  by going to higher-order approximations for  $R_0(\tau)$ .

#### E. Generalization to arbitrary angular momentum

The nonrelativistic generalization of the SVZ method to states with orbital angular momentum  $l > 0$  is based on the properties of the two-point functions for irreducible tensor currents  $T_{lm}(\nabla)$  (we again omit possible spin dependence). The scalar polarization function  $\Pi_l(E)$  satisfies a dispersion relation of the usual form with  $\text{Im}\Pi_l(E)$  proportional to the quantity

$$\lim_{r',r \rightarrow 0} \frac{1}{(r'r)^l} \sum_{n=1}^{\infty} R_{nl}(r') R_{nl}^*(r) \delta(E - E_{nl}), \quad (36)$$

where  $R_{nl}$  is the radial wave function for the  $n$ th state with angular momentum  $l$ . Repeated differentiation of the dispersion relation and application of the Borel transformation in Eq. (17) leads to an exponential-moment relation analogous to the  $S$ -wave relation in Eqs. (18)–(20),

$$\begin{aligned} \mathcal{X}_l(0,0,-i\tau) &= \lim_{r',r \rightarrow 0} \frac{1}{(r'r)^l} \sum_{n=1}^{\infty} R_{nl}(r') R_{nl}^*(r) e^{-E_{nl}\tau} \\ &\propto \int_0^{\infty} dE e^{-E\tau} W^2 \sigma_l(E). \end{aligned} \quad (37)$$

Here  $\sigma_l(E)$  is the cross section for the production of  $q\bar{q}$

bound states with angular momentum  $l$  through the action of the tensor current  $T_{lm}(\nabla)$ .

Equation (37) is of exactly the same form as Eqs. (19) or (20) [but with  $\mathcal{X}_0(0,0,-i\tau)=4\pi K(0,0,-i\tau)$ , an irrelevant change in normalization]. The energy  $E_{1l}$  is therefore given by the limit

$$E_{1l} = \lim_{\tau \rightarrow \infty} R_l(\tau), \quad (38)$$

where

$$R_l(\tau) = -\frac{d}{d\tau} \ln \mathcal{X}_l(0,0,-i\tau), \quad (39)$$

and we can use the criteria established in Sec. II C to obtain a best estimate for  $E_{1l}$  from the perturbation expansion of  $R_l(\tau)$ . We will restrict our discussion here to the first-order theory, and use the estimate

$$E_{1l}^{(1)} = \min_{\tau} [R_l^{(1)}(\tau)]. \quad (40)$$

The function  $(r'r)^l \mathcal{X}_l(r',r,-i\tau)$  is just the radial part of the Euclidean propagator for angular momentum  $l$ , and can be projected out of the full propagator

$$\begin{aligned} K(\vec{r}',\vec{r},-i\tau) &= \sum_{nlm} \psi_{nlm}(\vec{r}') e^{-E_{nl}\tau} \psi_{nlm}^*(\vec{r}) \\ &= \sum_{nlm} R_{nlm}(r') Y_{lm}(\hat{r}') e^{-E_{nl}\tau} R_{nlm}^*(r) Y_{lm}^*(\hat{r}) \end{aligned} \quad (41)$$

by using the orthogonality of the spherical harmonics  $Y_{lm}$ ,  $(r'r)^l \mathcal{X}_l(r',r,-i\tau)$

$$= \int d\Omega_{\hat{r}'} \int d\Omega_{\hat{r}} Y_{lm}^*(\hat{r}') K(\vec{r}',\vec{r},-i\tau) Y_{lm}(\hat{r}). \quad (42)$$

The result is independent of  $m$ . We can calculate the perturbation expansion of  $\mathcal{X}_l$  needed above by applying this operation to the usual series

$$K(\vec{r}',\vec{r},-i\tau) = K^{(0)}(\vec{r}',\vec{r},-i\tau) - \int_0^\tau d\tau' \int d^3r'' K^{(0)}(\vec{r}',\vec{r}'',-i(\tau-\tau')) V(r'') K^{(0)}(\vec{r}'',\vec{r},-i\tau') + \dots, \quad (43)$$

where

$$K^{(0)}(\vec{r}',\vec{r},-i\tau) = \left[ \frac{m_q}{4\pi\tau} \right]^{3/2} e^{-m_q(\vec{r}'-\vec{r})^2/4\tau}. \quad (44)$$

The angular integrals encountered in this calculation can be evaluated by using the expansion<sup>22</sup>

$$\begin{aligned} e^{m_q \vec{r}' \cdot \vec{r}' / 2\tau} &= \left[ \frac{\pi\tau}{m_q r r'} \right]^{1/2} \sum_{l=0}^{\infty} (2l+1) I_{l+1/2} \left[ \frac{m_q r r'}{2\tau} \right] P_l(\hat{r}' \cdot \hat{r}') \\ &= 4\pi \left[ \frac{\pi\tau}{m_q r r'} \right]^{1/2} \sum_{l=0}^{\infty} (2l+1) I_{l+1/2} \left[ \frac{m_q r r'}{2\tau} \right] Y_{lm}(\hat{r}') Y_{lm}^*(\hat{r}'). \end{aligned} \quad (45)$$

Here  $I_{l+1/2}$  is a hyperbolic Bessel function<sup>23</sup>

$$I_{l+1/2}(z) = \sum_{k=0}^{\infty} \frac{1}{k! \Gamma(k+m+\frac{3}{2})} \left[ \frac{z}{2} \right]^{m+1/2+2k}. \quad (46)$$

Dividing the result by  $(r'r)^l$  and taking the limit  $r',r \rightarrow 0$ , we find that

$$\mathcal{X}_l^{(0)}(0,0,-i\tau) = \frac{2}{\Gamma(l+\frac{3}{2})} \left[ \frac{m_q}{4\tau} \right]^{l+3/2} \quad (47)$$

and

$$\begin{aligned} \mathcal{X}_l^{(1)}(0,0,-i\tau) &= -\frac{4}{[\Gamma(l+\frac{3}{2})]^2} \int_0^\infty dr r^{2l+2} V(r) \int_0^\tau d\tau' \left[ \frac{m_q}{4(\tau-\tau')} \right]^{l+3/2} \left[ \frac{m_q}{4\tau'} \right]^{l+3/2} \\ &\quad \times \exp[-m_q r^2/4(\tau-\tau') - m_q r'^2/4\tau']. \end{aligned} \quad (48)$$

The integral over  $\tau'$  in Eq. (48) can be evaluated by repeated differentiation of the identity<sup>24</sup>

$$\int_0^\tau d\tau' \frac{1}{[(\tau-\tau')r']^{3/2}} e^{-x^2/(\tau-\tau') - x'^2/\tau'} = \frac{2\sqrt{\pi}}{\tau^{3/2}} \frac{1}{x} e^{-4x^2/\tau}, \quad (49)$$

and we find after some calculation that

$$\mathcal{X}_l^{(1)}(0,0,-i\tau) = -\mathcal{X}_l^{(0)}(0,0,-i\tau) \frac{m_q}{\Gamma(l+\frac{3}{2})} \int_0^\infty dr r V(r) e^{-m_q r^2/\tau} \sum_{k=0}^l \frac{l! \Gamma(l-k+\frac{1}{2})}{k!(l-k)!} \left[ \frac{m_q r^2}{\tau} \right]^k. \quad (50)$$

The perturbation expansion for  $R_l(\tau)$  is given to first order by

$$R_l^{(1)}(\tau) = -\frac{d}{d\tau} \ln[\mathcal{X}_l^{(0)}(0,0,-i\tau) + \mathcal{X}_l^{(1)}(0,0,-i\tau) + \dots] = \frac{l + \frac{3}{2}}{\tau} - \frac{d}{d\tau} (\mathcal{X}_l^{(1)}/\mathcal{X}_l^{(0)}). \quad (51)$$

Using the result in Eq. (50), we obtain our basic expression,

$$\begin{aligned} R_l^{(1)}(\tau) &= \frac{l + \frac{3}{2}}{\tau} + \frac{\sqrt{\pi}}{\Gamma(l + \frac{3}{2})} \frac{m_q^2}{\tau^2} \int_0^\infty dr r^3 V(r) e^{-m_q r^2/\tau} \sum_{k=0}^l \frac{l! \Gamma(l - k - \frac{1}{2})}{k! (l - k)! \Gamma(-\frac{1}{2})} \left[ \frac{m_q r^2}{\tau} \right]^k \\ &= \frac{l + \frac{3}{2}}{\tau} + \int_0^\infty dz H_l(z) V \left[ \left[ \frac{\tau z}{m_q} \right]^{1/2} \right], \quad z = m_q r^2/\tau. \end{aligned} \quad (52)$$

For  $l=0$ , this expression reduces to the  $S$ -wave result given in Eq. (31), and the estimate for the energy  $E_{1S}$  given by Eq. (40) is related to a variational principle as shown earlier. There is no generalization of the variational result for  $l > 0$ : The function  $H_l(z)$  which multiplies  $V$  in the integrand in Eq. (52) is negative for  $z \rightarrow 0$  and positive for  $z \rightarrow \infty$ , and cannot be interpreted as the square of a trial wave function.

#### F. A semiclassical result for $E_{1l}$

Although we do not have an analog of the variational result for  $E_{1S}$  for  $l > 0$ , we can derive an interesting first-order relation for  $E_{1l}$ ,  $l \geq 0$ , which relates the ground-state energies for different values of  $l$  (and  $m_q$ ) and shows why the generalized SVZ relations work. We begin by making an estimate of the integral in Eqs. (52). The function  $H_l(z)$  in the integral is peaked for  $z = m_q r^2/\tau$  slightly larger than  $l$  (see Fig. 1), has unit area, and can be approximated very roughly by a  $\delta$  function at  $z = l' \approx l$ . A good

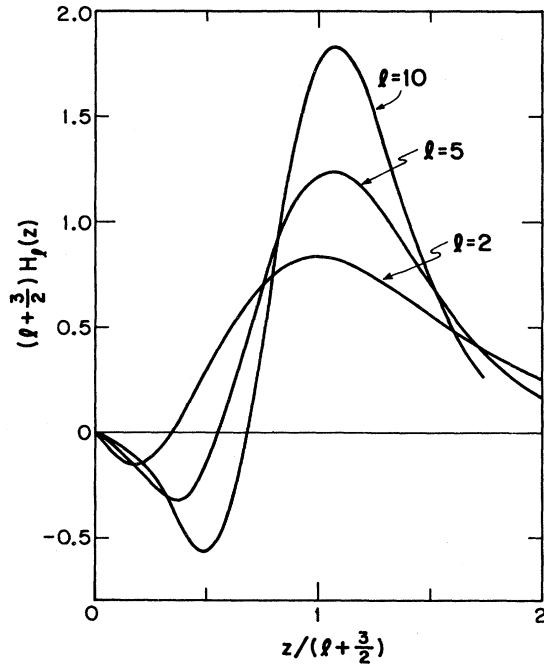


FIG. 1. Plot of the function  $(l + \frac{3}{2})H_l(z)$  defined in Eq. (52) as a function of the scaled variable  $z/(l + \frac{3}{2})$ .

approximation for power-law potentials gives  $l' \approx l + \frac{3}{2}$ . With this choice,

$$R_l^{(1)}(\tau) \approx \frac{l'}{\tau} + V \left[ \left[ \frac{l'\tau}{m_q} \right]^{1/2} \right]. \quad (53)$$

The approximation is surprisingly good for smooth potentials as we will see in the next section. More important for present purposes, Eq. (53) indicates the way in which  $R_l^{(1)}(\tau)$  changes with changes in  $l$  and  $m_q$ , and therefore allows us to relate the energies of different angular momentum states and different heavy-quark systems. For these relations to be reliable, the functional form of  $V(r)$  must not change rapidly between the regions of  $r$  which are most important in determining the energies we wish to relate. (This is the case for simple power-law potentials.)

If we now apply the criterion in Eq. (40) to determine a best value for the first-order energy  $E_{1l}^{(1)}$  for large  $l$ , we find that  $\tau_{\min}$  is determined by the equation

$$\begin{aligned} 0 &= \frac{d}{d\tau} R_l^{(1)}(\tau) \approx -\frac{l'}{\tau^2} + \frac{1}{2} \left[ \frac{l'}{m_q \tau} \right]^{1/2} V' \left[ \left[ \frac{l'\tau}{m_q} \right]^{1/2} \right] \\ &\approx \frac{1}{2} \frac{l'}{m_q r_0} \left[ -\frac{2l'}{m_q r_0^3} + V'(r_0) \right], \end{aligned} \quad (54)$$

$$r_0 = (l' \tau_{\min} / m_q)^{1/2}, \quad l' \approx l + \frac{3}{2}.$$

The vanishing of the function in the square brackets in Eq. (54) is just the condition that the classical effective potential

$$V_{\text{eff}}(r) = \frac{l'^2}{m_q r^2} + V(r) \quad (55)$$

have a minimum at the radius  $r = r_0$  (the condition for a stable circular orbit for classical angular momentum  $l + \frac{3}{2}$ ), and  $E_{1l}^{(1)}$  is approximated by the energy at the minimum,

$$E_{1l}^{(1)} \approx V_{\text{eff}}(r_0). \quad (56)$$

We can understand this unexpected result as follows: The Euclidean propagator  $K(\vec{r}', \vec{r}, -i\tau)$  is given by the Feynman path integral<sup>18</sup>

$$K(\vec{r}', \vec{r}, -i\tau) = \int_{\vec{r}}^{\vec{r}'} \mathcal{D}\vec{r}(\tau) \exp \left[ - \int_0^\tau H(\dot{\vec{r}}, \vec{r}) d\tau \right], \quad (57)$$

where  $H$  is the Hamiltonian of the system and the integral includes all paths which connect  $\vec{r}$  and  $\vec{r}'$  in "time"  $\tau$ . In calculating  $\mathcal{X}_l(0,0,-i\tau)$ , we restrict the paths to those

with classical angular momentum in a band around  $l$  by the projection in Eq. (42). Paths which reach the origin for  $l > 0$  must then tunnel through a classically forbidden region. The tunneling factors are divided out when we divide Eq. (42) by  $(r'r)^l$  and take the limit  $r', r \rightarrow 0$ . The leading contributions to  $\mathcal{X}_l(0, 0, -i\tau)$  arise from the paths on which  $H(\vec{r}, \vec{r})$  is a minimum subject to the tunneling constraints. In the approximation which leads to Eq. (56), we have in effect minimized  $\int_0^\tau H(\vec{r}, \vec{r}) d\tau$  for long times  $\tau$  by using the classical circular orbit for angular momentum  $l' \approx l + \frac{3}{2}$ , and have neglected quantum oscillations about the orbit and the effect of the potential on the tunneling. (The appearance of  $l'$  instead of  $l$  in  $r_0$  is ap-

parently connected with the increasing phase space available in the path integral for increasing  $r$ .) These approximations give

$$(r'r)^l \mathcal{X}_l(r', r, -i\tau) \propto (r'r) e^{-H_{\min} \tau} \quad (58)$$

and

$$-\frac{d}{d\tau} \ln \mathcal{X}_l(0, 0, -i\tau) \approx H_{\min} = E_{1l}^{(1)}. \quad (59)$$

The effect of localized radial oscillations about the classical path can be estimated by noting that Eq. (56) is an approximation to the JWKB expression for the energy. The JWKB quantization condition is

$$\left[ n + \frac{l}{2} - \frac{1}{4} \right] \pi = m_q^{1/2} \int dr [E_{nl} - V_{\text{eff}}(r)]^{1/2} \\ \approx m_q^{1/2} \int dr \left\{ [E_{nl} - V_{\text{eff}}(r_0)] + \frac{1}{2} V_{\text{eff}}''(r_0) (r - r_0)^2 \cdots \right\}^{1/2}, \quad (60)$$

and

$$E_{nl} \approx V_{\text{eff}}(r_0(l)) + (2n + l - \frac{1}{2}) [2V_{\text{eff}}''(r_0)/m_q]^{1/2}, \quad n = 1, 2, \dots, l \geq 1. \quad (61)$$

The result for  $E_{1l}$  in Eq. (56) follows if we can neglect the zero-point ( $n = 1$ ) energy of the radial oscillations.

We reemphasize at this point that Eq. (56) [or Eq. (61)] gives a useful relation between  $n = 1$  levels with different values of  $l$  whether the approximate energies are correct or not. We will in fact see in the next section that these relations give the proper JWKB  $l$  dependence of the ground-state energies for power-law potentials.

### III. NUMERICAL TESTS AND EXTENSION OF THE SVZ METHOD

#### A. First-order results for power-law potentials

It is straightforward to evaluate  $R_l^{(1)}(\tau)$  for a general power-law potential

$$V(r) = \int d\nu \rho(\nu) (r/a)^\nu, \quad \nu > -2 \quad (62)$$

by using the identity

$$H_l(z) = (-1)^{l+1} \frac{\Gamma(\frac{3}{2})}{\Gamma(l + \frac{3}{2})} z \frac{d}{dz} z^{l+1/2} \left[ \frac{d}{dz} \right]^l \frac{e^{-z}}{\sqrt{z}}, \quad (63)$$

which follows from Eqs. (48)–(51), and integrating repeatedly by parts in Eq. (52). The final integration gives a  $\Gamma$  function, and we find that

$$R_l^{(1)}(\tau) = \frac{l + \frac{3}{2}}{\tau} + \int d\nu \rho(\nu) \frac{\Gamma(\frac{3}{2}) \Gamma(l + \nu/2 + \frac{3}{2}) \Gamma(2 + \nu/2)}{\Gamma(\frac{3}{2} + \nu/2) \Gamma(l + \frac{3}{2})} \left[ \frac{\tau}{m_q a^2} \right]^{\nu/2}. \quad (64)$$

We will first consider the case of the simple power-law potential

$$V(r) = (\text{sgn } \nu) V_0 (r/a)^\nu, \quad V_0 > 0, \quad (65)$$

where we have chosen the sign of  $V(r)$  so that the potential supports bound states. It will be convenient to use a scaled time variable  $x = \lambda \tau$  and to express energies and  $R_l^{(1)}$  in units of  $\lambda$ , with

$$\lambda = V_0^{2/(2+\nu)} (m_q a^2)^{-\nu/(2+\nu)}. \quad (66)$$

Then with  $\mathcal{R}_l(x) = R_l(\tau)/\lambda$ , we have

$$R_l^{(1)}(x) = \frac{l + \frac{3}{2}}{x} + (\text{sgn } \nu) \frac{\Gamma(\frac{3}{2}) \Gamma(l + \nu/2 + \frac{3}{2}) \Gamma(2 + \nu/2)}{\Gamma(\frac{3}{2} + \nu/2) \Gamma(l + \frac{3}{2})} x^{\nu/2} \\ \approx \frac{l + \frac{3}{2}}{x} + (\text{sgn } \nu) \frac{\Gamma(\frac{3}{2}) \Gamma(2 + \nu/2)}{\Gamma(\frac{3}{2} + \nu/2)} [(l + \frac{3}{2}) x]^{\nu/2}. \quad (67)$$



The second form of this expression (obtained by using Stirling's approximation for the  $\Gamma$  function) has the  $l$  dependence predicted by the large- $l$  approximation in Eq. (53) (but with  $l \rightarrow l + \frac{3}{2}$ ). However, the magnitude of the second term in Eq. (67) is too small by 21% for  $\nu = -1$ , correct for  $\nu = 0$ , and too large by 18% and 33%, respectively, for  $\nu = 1$  and 2. These errors are  $l$  independent. Their pattern is easily deduced from the form of the function  $H_l(z)$  in the integral in Eq. (52) (see Fig. 1).

The value of the first-order energy  $E_{1l}^{(1)}$  is easily determined using Eqs. (40) and (67):

$$E_{1l}^{(1)} = \lambda(l + \frac{3}{2})(1 + 2/\nu) [\frac{1}{2} |\nu| C(\nu)]^{2/(\nu+2)}, \quad \nu > -2 \quad (68)$$

where

$$C(\nu) = \frac{\Gamma(\frac{3}{2})\Gamma(l + \nu/2 + \frac{3}{2})\Gamma(2 + \nu/2)}{\Gamma(\frac{3}{2} + \nu/2)\Gamma(l + \frac{5}{2})} \approx \frac{\Gamma(\frac{3}{2})\Gamma(2 + \nu/2)}{\Gamma(\frac{3}{2} + \nu/2)} (l + \frac{3}{2})^{\nu/2 - 1}. \quad (69)$$

If we use the approximate form of  $C(\nu)$  in Eq. (68), we obtain the semiclassical scaling law for  $E_{1l}^{(1)}$  implied by Eq. (56):

$$E_{1l}^{(1)} = \lambda(1 + 2/\nu) \left[ \frac{|\nu| \Gamma(\frac{3}{2})\Gamma(2 + \nu/2)}{2\Gamma(\nu/2 + \frac{3}{2})} \right]^{2/(\nu+2)} \times (l + \frac{3}{2})^{2\nu/(\nu+2)}. \quad (70)$$

The  $l$  dependence of this expression is just that obtained for  $n=1$  from the general JWKB expressions given by Quigg and Rosner<sup>25</sup>:

$$E_{nl}^{\text{JWKB}} = \lambda \left[ \frac{\Gamma(\frac{1}{2})\Gamma(\frac{3}{2} + 1/\nu)}{\Gamma(1 + 1/\nu)} \right]^{2\nu/(2+\nu)} \times (2n + l - \frac{1}{2})^{2\nu/(2+\nu)}, \quad \nu > 0, n = 1, 2, \dots \quad (71)$$

$$E_{nl}^{\text{JWKB}} = \lambda \left[ \frac{\Gamma(\frac{1}{2})\Gamma(1 - 1/\nu)}{\Gamma(\frac{1}{2} - 1/\nu)} \right]^{2\nu/(2+\nu)} \times (2n + l - \frac{1}{2} + \nu/2)^{2\nu/(2+\nu)}, \quad \nu < 0, n = 1, 2, \dots \quad (72)$$

provided we neglect the  $\nu/2$  in the last line of Eq. (72). The overall coefficient in Eq. (70) differs from the coefficients in Eqs. (71) and (72), but this difference is independent of  $l$ . The scaling of the energies with the potential strength and the quark mass is the same in all expressions, and is determined by Eq. (66).

The accuracy (or inaccuracy) of the first-order energies  $E_{1S}^{(1)}$  is shown in Figs. 2 and 3 where we compare the prediction of Eq. (70) with the Quigg-Rosner JWKB predictions from Eqs. (70) and (71), the higher-order predictions

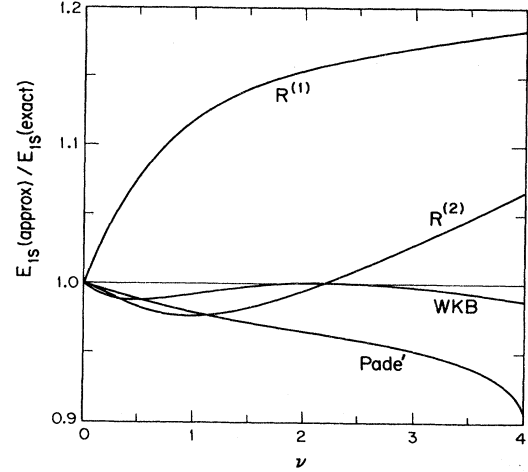


FIG. 2. Plots of the ratio of the approximate 1S energy to the exact energy for the confining power-law potential  $V(r) = V_0(r/a)^\nu$ ,  $V_0 > 0$ ,  $\nu > 0$ . The curves give the results obtained using the first-order and second-order exponential moments, Padé resummation of the second-order series, and the modified JWKB formula of Quigg and Rosner (Ref. 25).

which we will discuss in the following sections. As may be seen from the figures, the first-order result for  $E_{1S}$  is generally poor except for  $|\nu|$  quite small. The accuracy of the predicted ground-state energies  $E_{1l}$  for higher  $l$  is essentially the same as for  $E_{1S}$  because of the correct JWKB scaling in  $l$  given by Eq. (70). We note in this connection that if we were to scale the potential strength  $V_0$  in Eq. (65) by hand so that we fit  $E_{1S}$  exactly, we would obtain a good simultaneous fit to *all* the energies  $E_{1l}$ . However, it would clearly be incorrect to conclude from the accuracy of the overall fit either that the first-order method was accurate, or that the value of  $V_0$  determined in the fit was correct. This remark has obvious implications for the SVZ program, to which we will return.

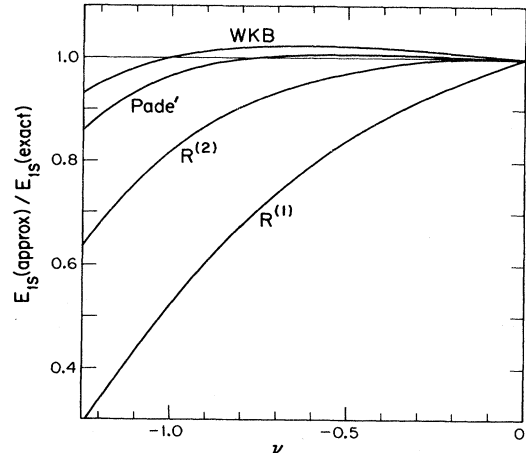


FIG. 3. Plots of the ratio of the approximate 1S energy to the exact energy for the attractive power-law potential  $V(r) = -V_0(r/a)^\nu$ ,  $V_0 > 0$ ,  $\nu < 0$ . The curves give the results obtained using the first-order and second-order exponential moments, Padé resummation of the second-order series, and the modified JWKB formula of Quigg and Rosner (Ref. 25).

The first-order predictions for  $E_{1l}$  are also quite poor for the realistic Coulomb-plus-linear potential used in fits to heavy-quarkonium systems,

$$V(r) = -\frac{a}{r} + br. \quad (73)$$

In this case  $R_l^{(1)}$  is given by the sum

$$R_l^{(1)}(\tau) = \frac{l + \frac{3}{2}}{\tau} - \frac{\pi a}{4} \frac{\Gamma(l+1)}{\Gamma(l + \frac{3}{2})} \left[ \frac{m_q}{\tau} \right]^{1/2} + \frac{3\pi b}{8} \frac{\Gamma(l+2)}{\Gamma(l + \frac{3}{2})} \left[ \frac{\tau}{m_q} \right]^{1/2}, \quad (74)$$

and the energies must be determined numerically.

Miller and Olsson<sup>26</sup> obtain a best fit to the spin-averaged charmonium and  $b$ -quarkonium data for  $m_c = 1.35$  GeV,  $m_b = 4.77$  GeV,  $a = 0.49$ , and  $b = 0.17$  GeV<sup>2</sup>. Using these parameters, we find the results given in Table II. We find, for example, that the predicted  $S$ - and  $P$ -state energies in charmonium are too large by 144 and 142 MeV, respectively, errors which are quite large on the scale of the absolute energies or the level spacing  $E_{1P} - E_{1S} = 408$  MeV. The latter is given essentially correctly,  $E_{1P}^{(1)} - E_{1S}^{(1)} = 406$  MeV. There are similar discrepancies in  $b$ -quarkonium.

We can force a fit to the exact charmonium energies by increasing the parameter  $a$  by 36% to  $a = 0.665$  and decreasing  $b$  by 16% to  $b = 0.146$  GeV<sup>2</sup>, and obtain at the same time remarkable improvements in the  $b$ -quarkonium energies. However, the potential which results is certainly not a good approximation to the input potential.

We can also greatly improve the (apparent) match of the

first-order and exact results for the *total* energies  $M_{1l} = E_{1l} + 2m_q$  simply by adjusting the quark masses downward by  $\sim 70$  MeV for charmonium and  $\sim 100$  MeV for  $b$ -quarkonium, again with misleading results (especially so if one looks only at the fractional error in  $M_{1l}$ ).

We conclude on the basis of these examples (and our earlier theoretical considerations) that the first-order predictions for the bound-state energies  $E_{1l}$  can be expected to be qualitatively correct, for example, to reflect the correct pattern of level spacings, but that the quantitative predictions for a given potential are unreliable. Conversely, potential parameters (or quark masses) determined by *forcing* the first-order energies to fit a given spectrum are likely to be substantially in error. This was pointed out for the  $S$  states by Bell and Bertlmann<sup>4,5</sup> who showed that the gluon-condensate parameter  $\phi_1$  in the SVZ effective potential<sup>6</sup>

$$V(r) = -\frac{4\alpha_s}{3r} + \frac{1}{64} m_q \phi_1 r^4 \quad (75)$$

is underestimated by a factor of 2 in fits to  $E_{1S}$  in charmonium. We will discuss the implications of these results in more detail later.

#### B. Extension of the SVZ method to higher order

Because of the difficulties with the first-order SVZ method discussed above, we have extended our analysis of the  $S$ -state problem to second order for the general power-law potential defined in Eq. (62), and to higher order in some special cases. The second-order result for  $R_0(\tau)$  follows easily from the corresponding expansion of the Euclidean propagator  $K(0,0,-i\tau)$  given in the preceding paper [WDD (Ref. 16)]:

$$R_0^{(2)}(\tau) = \frac{3}{2\tau} + \int d\nu_1 \rho(\nu_1) \Gamma \left[ 2 + \frac{\nu_1}{2} \right] \left[ \frac{\tau}{m_q a^2} \right]^{\nu_1/2} - \int d\nu_2 \rho(\nu_2) \int d\nu_1 \rho(\nu_1) \left[ 1 + \frac{\nu_1}{4} + \frac{\nu_2}{4} \right] \left\{ \Gamma \left[ 1 + \frac{\nu_1}{2} + \frac{\nu_2}{2} \right] \left[ \frac{\nu_1 + \nu_2 + 2}{(\nu_1 + 1)(\nu_2 + 1)} - \frac{\Gamma(\nu_1 + 1)\Gamma(\nu_2 + 1)}{\Gamma(\nu_1 + \nu_2 + 2)} \right] - \Gamma \left[ 1 + \frac{\nu_1}{2} \right] \Gamma \left[ 1 + \frac{\nu_2}{2} \right] \right\} \left[ \frac{\tau}{m_q a^2} \right]^{(2 + \nu_1 + \nu_2)/2} \tau. \quad (76)$$

This expression simplifies somewhat for a single power, i.e., the potential in Eq. (65). It is convenient in that case to use the scaled time variable  $x = \lambda\tau$  and the scaled function  $\mathcal{R}_0^{(2)} = R_0^{(2)}/\lambda$  with  $\lambda$  defined as in Eq. (66), and rewrite Eq. (76) as

$$\mathcal{R}_0^{(2)}(x) = \frac{3}{2x} + (\text{sgn } \nu) \Gamma \left[ 2 + \frac{\nu}{2} \right] x^{\nu/2} - B_\nu x^{\nu+1}, \quad (77)$$

where

$$B_\nu = (2 + \nu) \left\{ \Gamma(\nu + 1) \left[ \frac{1}{\nu + 1} - \frac{\Gamma^2(\nu + 1)}{2\Gamma(2\nu + 2)} \right] - \frac{1}{2} \Gamma^2 \left[ 1 + \frac{\nu}{2} \right] \right\}. \quad (78)$$

$B_\nu$  is positive in the region of interest ( $\nu > -2$ ), and has a quadratic zero at  $\nu=0$ .

We can obtain a second-order estimate for the ground-state energy  $E_{1S}$  by minimizing  $\mathcal{R}_0^{(2)}(x)$  with respect to  $x$  for  $-2 < \nu < -0.36918\dots$ . However, for  $\nu > -0.36918\dots$  no minimum exists, and we will therefore use the inflection-point criterion discussed following Eq. (29) and estimate  $E_{1S}$  as

$$E_{1S}^{(2)} = \lambda \mathcal{R}_0^{(2)}(x_{\text{inf}}), \quad (79)$$

where

$$\frac{d^2}{dx^2} \mathcal{R}_0^{(2)}(x_{\text{inf}}) = 0. \quad (80)$$

After some calculation, we find that

$$E_{1S}^{(2)} = \lambda \mathcal{R}_0^{(2)}(\hat{x}), \quad (81)$$

where

$$\hat{x}^{1+\nu/2} = \left\{ \frac{|\nu|}{2} \Gamma \left[ 2 + \frac{\nu}{2} \right] - \left[ \frac{1}{4} \nu^2 \Gamma^2 \left[ 2 + \frac{\nu}{2} \right] - 6(\nu+1)B_\nu \right]^{1/2} \right\} / (\nu+1)B_\nu, \quad \nu < -0.36918\dots \quad (82)$$

and

$$\hat{x}^{1+\nu/2} = \left\{ \frac{|\nu|}{2} \left[ \frac{\nu}{2} - 1 \right] \Gamma \left[ 2 + \frac{\nu}{2} \right] + \left[ \frac{\nu^2}{4} \left[ \frac{\nu}{2} - 1 \right]^2 \Gamma^2 \left[ 2 + \frac{\nu}{2} \right] + 12\nu(\nu+1)B_\nu \right]^{1/2} \right\} / \nu(\nu+1)B_\nu, \quad \nu > -0.36918\dots \quad (83)$$

To check the theoretical reliability of the minimum and inflection-point criteria for determining the optimum choice of  $\hat{x}$ , we have applied these methods for the Coulomb, linear, and oscillator potentials using the following extended results obtained in WDD (Refs. 16 and 27):

$\nu = -1$ :

$$K(0,0,-i\tau) = 4\sqrt{\pi} \left[ \frac{m_q}{4\pi\tau} \right]^{3/2} \sum_{n=0}^{\infty} \frac{\zeta(n)}{\Gamma[(n-1)/2]} \left[ \frac{x}{4} \right]^{n/2} \\ = \left[ \frac{m_q}{4\pi\tau} \right]^{3/2} \left[ 1 + \sqrt{\pi}x^{1/2} + \frac{\pi^2}{6}x + \frac{1}{2}\sqrt{\pi}\zeta(3)x^{3/2} + \frac{\pi^4}{180}x^2 + \dots \right], \quad (84)$$

$$\mathcal{R}_0(x) = \frac{3}{2x} - \frac{1}{2}\sqrt{\pi}x^{-1/2} - \frac{\pi}{6}(\pi-3) - \frac{3}{4}\sqrt{\pi} \left[ \zeta(3) + \frac{2\pi}{3} - \frac{\pi^2}{3} \right] x^{1/2} + \frac{\pi}{2} \left[ \frac{\pi^3}{30} - \frac{2\pi^2}{3} + 2\zeta(3) + \pi \right] x^{3/2} + \dots \quad (85)$$

$\nu = +1$ :

$$K(0,0,-i\tau) = \left[ \frac{m_q}{4\pi\tau} \right]^{3/2} \left[ 1 - \frac{\sqrt{\pi}}{2}x^{3/2} + \frac{5}{12}x^3 - \frac{5\sqrt{\pi}}{64}x^{9/2} + \frac{221}{6048}x^6 - \dots \right], \quad (86)$$

$$\mathcal{R}_0(x) = \frac{3}{2x} + \frac{3\sqrt{\pi}}{4}x^{3/2} + \frac{1}{8}(3\pi-10)x^3 + \frac{3\sqrt{\pi}}{16}(\pi - \frac{25}{8})x^{9/2} + \frac{1}{32} \left[ 3\pi^2 - \frac{25\pi}{2} + \frac{608}{63} \right] x^6 + \dots, \quad (87)$$

$\nu = +2$ :

$$K(0,0,-i\tau) = \left[ \frac{m_q}{4\pi\tau} \right]^{3/2} \left[ \frac{2x}{\sinh 2x} \right]^{3/2} = \left[ \frac{m_q}{4\pi\tau} \right]^{3/2} (1 - x^2 + \frac{19}{30}x^4 - \frac{631}{1890}x^6 + \frac{1219}{7560}x^8 - \dots), \quad (88)$$

$$\mathcal{R}_0(x) = 3 \coth 2x = \frac{3}{2x} \sum_{n=0}^{\infty} \frac{B_{2n}}{(2n)!} (4x)^{2n} = \frac{3}{2x} + 2x - \frac{8}{15}x^3 + \frac{64}{315}x^5 - \frac{128}{1575}x^7 + \dots, \quad (89)$$

where  $B_n$  is the  $n$ th Bernoulli number. It is interesting to note that the contributions of the second- and higher-order terms are much suppressed in  $\mathcal{R}_0$  (even more so in  $-\ln K$ ) relative to  $K$ , as would be expected from the arguments in Ref. 19.

We show our high-order results for the oscillator and Coulomb potentials in Figs. 4 and 5. The validity of the minimum and inflection-point criteria for determining the optimum estimate for  $E_{1S}^{(n)}$  from  $\mathcal{R}_0^{(n)}(x)$  is clearly evident from these figures. We emphasize that the sequence of

optimum values converges to the exact function  $\mathcal{R}_0(x)$  evaluated for  $x = x_{\text{optimum}}$ , and not to  $E_{1S} = \mathcal{R}_0(\infty)$ . It is necessary to estimate the contributions of higher states to  $\mathcal{R}(x)$  if one is to correct for this effect. The curves in Figs. 4 and 5 show that the estimates for  $E_{1S}$  can be improved substantially by including second- or higher-order terms in  $\mathcal{R}_0(x)$ , but illustrate also that the convergence of the perturbation series is sufficiently slow that it is probably not worthwhile to go beyond second order. (Even going to second order would require a major effort in the

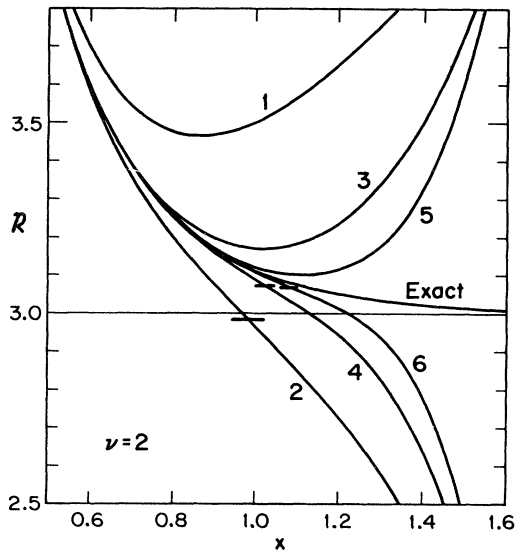


FIG. 4. Convergence of the  $n$ th-order approximations  $\mathcal{R}_0^{(n)}(x)$  to the exact moment function  $\mathcal{R}_0(x) = 3 \coth 2x$  for the oscillator potential. The short horizontal bars show the optimum values of  $\mathcal{R}_0^{(n)}(x)$  for  $n=2, 4, 6$  determined by the inflection-point criterion of Sec. II C. The optimum values of  $\mathcal{R}_0^{(n)}(x)$  for  $n=1, 3, 5$  are given by the minima of the corresponding curves.

field-theoretic context.)

In Figs. 6–11, we show the behavior of the functions  $\mathcal{R}_0^{(1)}(x)$  and  $\mathcal{R}_0^{(2)}(x)$  for simple power-law potentials with  $\nu=2, 1, \frac{1}{2}, -\frac{1}{2}, -1$ , and for the realistic Coulomb-plus-linear potential with the parameters of Ref. 26. The first-order estimates of  $E_{1S}$  given by the minima in the curves are unreliable as noted earlier. The second-order estimates are much improved in all cases. The necessity of having an analytic criterion to pick the optimal value of  $\mathcal{R}_0^{(2)}(x)$  for  $\nu > -0.36918 \dots$  is clearly evident from Figs. 6–8 and 11.<sup>28</sup>

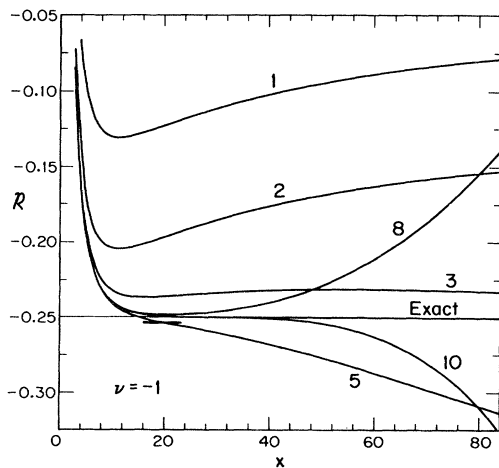


FIG. 5. Convergence of the  $n$ th-order approximations  $\mathcal{R}_0^{(n)}(x)$  to the exact moment function  $\mathcal{R}_0(x)$  for the Coulomb potential. The optimum values of  $\mathcal{R}_0^{(n)}(x)$  are at the minima of the curves for  $n=1, 2, 3$ , and 8, and at the inflection point indicated by the horizontal bar for  $n=5$ .

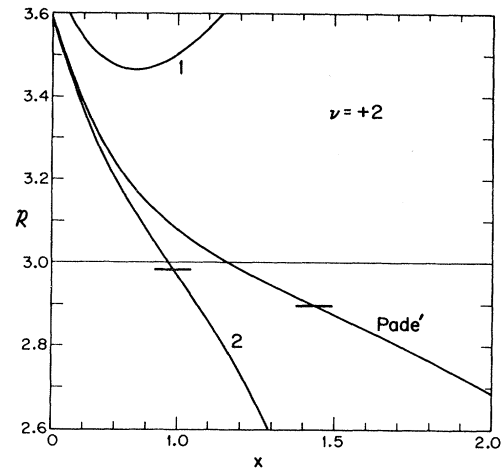


FIG. 6. Behavior of the first- and second-order exponential moment functions  $\mathcal{R}_0^{(1)}(x)$  and  $\mathcal{R}_0^{(2)}(x)$  and the Padé modification of  $\mathcal{R}_0^{(2)}(x)$  for  $\nu = +2$ . The horizontal bars indicate the optimum values of  $\mathcal{R}_0$  determined by the inflection-point criterion. The horizontal line gives the exact value of  $\mathcal{R}_0(\infty)$ .

The overall accuracy of the first- and second-order estimates of  $E_{1S}$  for power-law potentials is shown for  $-1.25 < \nu < 4$  in Figs. 2 and 3. It is encouraging that the second-order results are nearly as good as the JWKB results of Quigg and Rosner<sup>25</sup> for  $-\frac{1}{2} \leq \nu \leq \frac{5}{2}$ , and are reasonably accurate even for  $\nu=4$ . However, there are still problems in the interesting region  $\nu \sim -1$ . We therefore consider the possibility of improving the convergence of the perturbation series using Padé resummation.<sup>29</sup>

### C. Padé summation

The Padé summation technique approximates the partial sums of a power series by a ratio of polynomials. If the first  $m + n + 1$  terms of the series

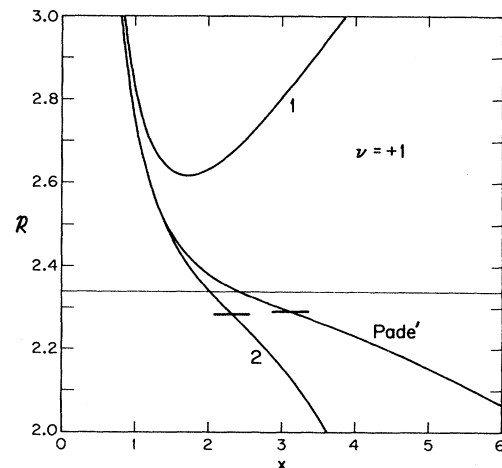


FIG. 7. Behavior of the first- and second-order exponential moment functions  $\mathcal{R}_0^{(1)}(x)$  and  $\mathcal{R}_0^{(2)}(x)$  and the Padé modification of  $\mathcal{R}_0^{(2)}(x)$  for  $\nu = +1$ . The horizontal bars indicate the optimum values of  $\mathcal{R}_0$  determined by the inflection-point criterion. The horizontal line gives the exact value of  $\mathcal{R}_0(\infty)$ .

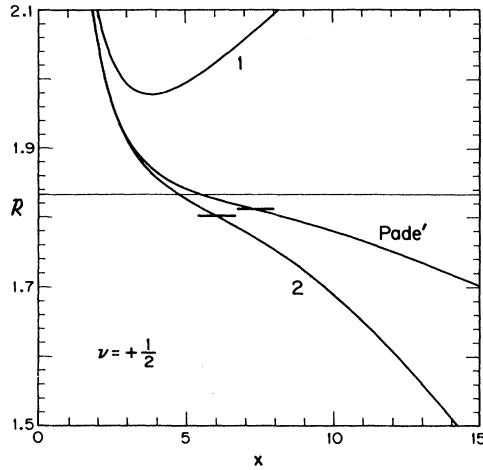


FIG. 8. Behavior of the first- and second-order exponential moment functions  $\mathcal{R}_0^{(1)}(x)$  and  $\mathcal{R}_0^{(2)}(x)$  and the Padé modification of  $\mathcal{R}_0^{(2)}(x)$  for  $\nu = +\frac{1}{2}$ . The horizontal bars indicate the optimum values of  $\mathcal{R}_0$  determined by the inflection-point criterion. The horizontal line gives the exact value of  $\mathcal{R}_0(\infty)$ .

$$P^{(n+m)} = \sum_{j=0}^{m+n} a_j z^j \quad (90)$$

are known, the  $[n, m]$  Padé approximant for  $P$  is the ratio

$$P[n, m] = \left[ \sum_{j=0}^n N_j z^j \right] / \left[ 1 + \sum_{j=1}^m D_j z^j \right], \quad (91)$$

where the coefficients  $N_j$  and  $D_j$  are determined by the condition that the expanded form of  $P[n, m]$  reproduce the series to order  $z^{n+m}$ . It can be shown for many types of series that the sequence of Padé approximants converges to the function defined by the original series for

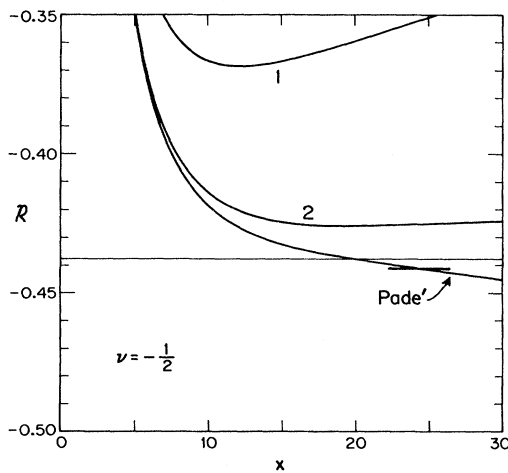


FIG. 9. Behavior of the first- and second-order exponential moment functions  $\mathcal{R}_0^{(1)}(x)$  and  $\mathcal{R}_0^{(2)}(x)$  and the Padé modification of  $\mathcal{R}_0^{(2)}(x)$  for  $\nu = -\frac{1}{2}$ . The horizontal bar indicates the optimum value of  $\mathcal{R}_0^{\text{Padé}}$  determined by the inflection-point criterion. The horizontal line gives the exact value of  $\mathcal{R}_0(\infty)$ .

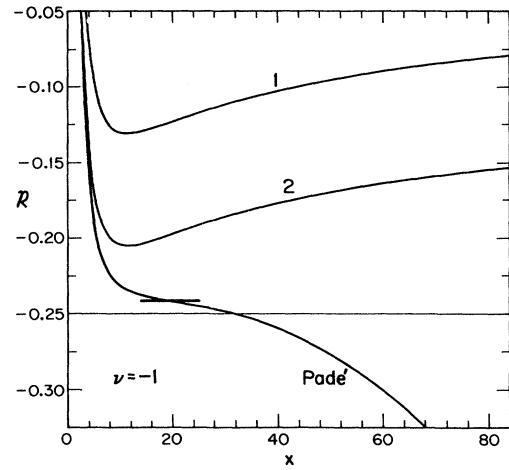


FIG. 10. Behavior of the first- and second-order exponential moment functions  $\mathcal{R}_0^{(1)}(x)$  and  $\mathcal{R}_0^{(2)}(x)$  and the Padé modification of  $\mathcal{R}_0^{(2)}(x)$  for  $\nu = -1$ . The horizontal bar indicates the optimum value of  $\mathcal{R}_0^{\text{Padé}}$  determined by the inflection-point criterion. The horizontal line gives the exact value of  $\mathcal{R}_0(\infty)$ .

$n, m \rightarrow \infty$ , and moreover, that the convergence is more rapid and the region of convergence larger than for the original series.<sup>29</sup> In essence, the Padé representation approximates the smoothly varying part of the series by the smoothly varying ratio of two polynomials.

We have applied the Padé technique to  $\mathcal{R}_0^{(2)}(x)$ , Eq. (77), by writing this function as

$$\mathcal{R}_0^{(2)}(x) = \frac{1}{x} P^{(2)}(x^{1+\nu/2}) \quad (92)$$

and constructing a  $[1, 1]$  approximant for  $P^{(2)}$  in the variable  $x^{1+\nu/2}$ ,

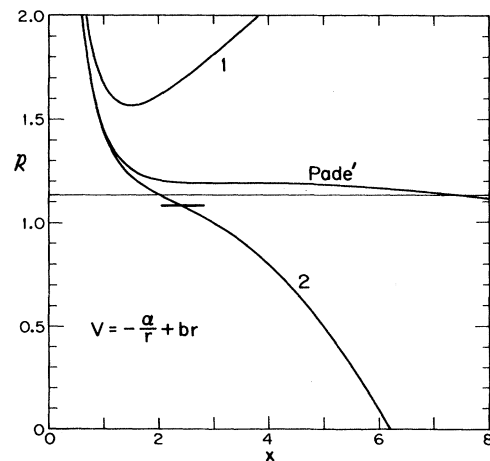


FIG. 11. Behavior of the first- and second-order exponential moment functions  $\mathcal{R}_0^{(1)}(x)$  and  $\mathcal{R}_0^{(2)}(x)$  and the Padé modification of  $\mathcal{R}_0^{(2)}(x)$  for the Coulomb-plus-linear potential  $V(r) = -ar^{-1} + br$  with parameters  $a = 0.49$ ,  $b = 0.17 \text{ GeV}^2$  chosen to fit the spin-averaged charmonium spectrum (Ref. 26). The variable  $x$  is scaled using the scaling for a linear potential. The horizontal line gives the exact value of  $\mathcal{R}_0(\infty)$ .

$$P^{(2)} \rightarrow P[1,1] = \frac{\frac{3}{2} + N_1 x^{1+\nu/2}}{1 + D_1 x^{1+\nu/2}}, \quad (93)$$

where

$$N_1 = (\text{sgn } \nu) \left[ \Gamma \left[ 2 + \frac{\nu}{2} \right] + B_\nu / \Gamma \left[ 2 + \frac{\nu}{2} \right] \right] \quad (94)$$

and

$$D_1 = (\text{sgn } \nu) B_\nu / \Gamma \left[ 2 + \frac{\nu}{2} \right]. \quad (95)$$

The optimum values of  $x$  and  $\mathcal{R}_0^{(2)}$  were then obtained for  $x > -1.2$  using the inflection-point criterion. The Padé approximations to  $\mathcal{R}_0^{(2)}(x)$  for power-law potentials and the Coulomb-plus-linear potential are shown in Figs. 6–11.<sup>30</sup>

The accuracy of the Padé method relative to other methods is shown in Figs. 2 and 3. We see that the Padé method gives substantial improvements in the estimate of  $E_{15}$  for singular potentials. Thus for the Coulomb potential, the Padé estimate of  $E_{15}$  is only in error by 3.5% while the first- and second-order estimates are in error by 48% and 18%. On the other hand, there is no improvement in the energy estimates for  $\nu > 0$ . This difference reflects the fact that the series for  $\mathcal{R}_0(x)$  for the singular potentials have a number of slowly convergent terms with the same signs which are efficiently summed by the Padé technique. The alternating series which appear for  $\nu > 0$  are more sensitive to cancellations, and are summed less accurately.

We conclude that the Padé method can be applied to considerable advantage for realistic singular interactions, but that the simple second-order method is adequate for nonsingular interactions.

#### D. Determining the effective QCD potential

Bell and Bertlmann<sup>6</sup> showed that one can associate the small- $\tau$  expansion of  $R_0(\tau)$  obtained as the nonrelativistic limit of the SVZ expansion with an effective confining Coulomb-plus-quartic potential

$$V(r) = -\frac{4\alpha_s}{3r} + \frac{1}{64} m_q \phi_1 r^4 \quad (96)$$

in the sense that  $R_{\text{BB}}^{(1)}(\tau) = R_{\text{SVZ}}^{(1)}(\tau)$ . However, the quartic behavior of this potential at large  $r$  and the flavor dependence generated by the quark mass in the quartic term are in conflict with the many successful potential-theory results obtained for charmonium and  $b$ -quarkonium. It is therefore important to recognize that one *cannot* use the first-order SVZ procedure with the leading terms in the operator-product expansion to determine the nature of the *long-range* confining interaction in  $q\bar{q}$  systems. To illustrate this, we consider the hypothetical potential

$$V(r) = -\frac{4\alpha_s}{3r} + \frac{1}{16} m_q [(1 + \phi_1 r^4)^{1/4} - 1] \rightarrow \begin{cases} -\frac{4\alpha_s}{3r} + \frac{1}{64} m_q \phi_1 r^4 - \frac{3}{512} m_q \phi_1^2 r^4 + \dots, & \phi_1 r^4 \ll 1, \\ -\frac{4\alpha_s}{3r} + \frac{1}{16} m_q \phi_1^{1/4} r, & \phi_1 r^4 \gg 1. \end{cases} \quad (97)$$

This potential has the Bell-Bertlmann Coulomb-plus-quartic behavior for  $r$  small, but for the parameters used by those authors, is very nearly a (flavor-dependent) Coulomb-plus-linear potential in the region which is relevant for charmonium. The predicted energies are very different for the two potentials.

The exponential-moment function for the potential in Eq. (97) behaves for  $\tau \rightarrow 0$  as

$$R_0^{(1)}(\tau) = \frac{3}{2\tau} + \frac{3}{32} m_q \phi_1 \left[ \frac{\tau}{m_q} \right]^2 - \frac{45}{64} m_q \phi_1^2 \left[ \frac{\tau}{m_q} \right]^4 + \dots \quad (98)$$

The term linear in  $\phi_1$  gives the leading (nonrelativistic) dimension-four term in  $R_0^{(1)}(\tau)$ . The term proportional to  $\phi_1^2$  is of dimension eight, and is therefore nonleading in the sense of the operator-product expansion, and would have been omitted in the calculations carried out to date. Since Flory<sup>31</sup> has recently produced a potential of this more complicated sort by summing the gluon-condensate terms to all orders in an ultralocal, large- $N_c$  approximation, the ambiguity noted here may not be entirely hypothetical, and it will be important to extend the operator-product expansion to include higher-dimension operators.

The limitations of the SVZ approach for determining  $V(r)$ <sup>6</sup> and the energies of excited states<sup>4</sup> are rather striking when it is compared to the inverse scattering method of potential theory. In the latter, information on, e.g., a set of  $S$ -state energies can be used to construct an approximate potential which can then be used with the Schrödinger equation to predict the energies of states with  $l \neq 0$ . There is no (practical) restriction to ground-state energies  $E_{1l}$ . This procedure is quite successful for charmonium and  $b$ -quarkonium.<sup>26,32</sup> Unfortunately, no analog is known which is appropriate to the general field-theoretic problem.

#### E. Summary and implications for the SVZ program

In this paper we have investigated the theoretical foundations of the SVZ approach to the prediction of hadronic masses in QCD, modeling the SVZ procedure using nonrelativistic potential models. The relevance of these models to heavy-quark systems was established by Bertlmann<sup>3</sup> who showed that the predictions of the nonrelativistic and relativistic versions of the SVZ procedure agreed quite well with each other for charmonium and  $b$ -quarkonium. We believe that our general theoretical conclusions are also applicable to light-quark systems.

Our results show how the first-order SVZ method can work as well as it seems to in correlating hadronic masses, but still be unreliable in other applications, e.g., in predicting masses from known QCD parameters, or determining those parameters from fits to hadronic data. Our principal results are as follows.

(1) The first-order calculation of the  $S$ -wave energy  $E_{1S}$  using the SVZ exponential moments is quasivariational, and gives the best value of  $E_{1S}$  which can be obtained with the given input and method. The unexpected success of the SVZ procedure in extracting large- (Euclidean-) time results from a perturbation expansion valid at short times is a consequence of the hidden variational nature of the calculation. The predicted energy always lies above the true energy,  $E_{1S}^{(1)} > E_{1S}$ . As a result, the value of the gluon-condensate parameter  $\phi_1$  in the effective quark-antiquark potential<sup>6</sup> in Eq. (75) will always be *underestimated* if it is adjusted so that  $E_{1S}^{(1)}$  matches the correct energy. This effect was found by Bell and Bertlmann<sup>4</sup> in their numerical studies of power-law potentials, and was also shown to occur in the  $1/N_c$  expansion in two-dimensional QCD by Bradley *et al.*<sup>33</sup> and by Ditsas and Shaw.<sup>34</sup> Miller and Olsson<sup>35</sup> have recently concluded on purely phenomenological grounds that  $\phi_1$  was underestimated by SVZ and RRY. Their analysis of the charmonium data using finite-energy sum rules gave a value of  $\phi_1$  a factor of 2 larger than that obtained in the fits to  $E_{1S}$ .

We emphasize that the contribution of higher bound states (or the continuum) to the exact  $\mathcal{R}_0$  does not account for the difference between the first-order and exact values for  $E_{1S}$ . As shown in Figs. 4 and 5, the minimum values of  $\mathcal{R}_0^{(1)}$  for the oscillator and Coulomb potentials lie substantially above the exact values of  $\mathcal{R}_0$  at the same points. The “continuum” corrections may be important in some cases<sup>2</sup> but the basic problem remains.

(2) The first-order predictions for the ground-state energies  $E_{1l}$  for different angular momentum series are connected by an approximate semiclassical relation (precisely the JWKB relation up to an overall normalization for simple power-law potentials) which guarantees that the ener-

gies scale properly with the quark mass, and that an *entire set* of levels will be fitted reasonably well if the potential is adjusted to fit the lowest levels. A striking example of this phenomenon for the Coulomb-plus-linear potential is shown in Table II.

(3) *Conversely, success in fitting an entire complex of energy levels* (e.g., the spin-averaged charmonium and  $b$ -quarkonium levels in Table II) *does not guarantee that the potential parameters obtained in the fit are correct.* We conclude by analogy that the spectacular success of SVZ,<sup>1</sup> RRY,<sup>2</sup> and others<sup>3,36</sup> in fitting a large number of hadronic masses is essentially unrelated to the correctness of the QCD condensate derived in these fits. The situation is further complicated by the presence of extra adjustable parameters—quark masses, the quark condensate used in fits to light-quark data, etc.—which make definitive comparisons between different systems difficult. The clearest test of the method is probably the calculation of spin splittings within a given system. These depend on the condensates as well as the single-gluon-exchange terms, hence test the theoretical input. The results are only moderately successful.<sup>2,3</sup>

(4) The second-order predictions for  $E_{1S}$  appear to be quite reliable for a variety of potentials, especially if supplemented by Padé summation in the case of singular interactions. Use of the higher-order expressions in field-theoretic calculations would require that the operator-product expansion be extended to include higher-dimensional operators (the gluon condensate appears quadratically in dimension eight). Considerable progress on this task has been made recently by Nikolaev and Radyushkin.<sup>37</sup> We emphasize that it is only with the use of such higher-order methods that one can hope to obtain reliable values for the nonperturbative condensate parameters, e.g., for comparison to the results of lattice calculations. We remark finally that high-order calculations are also required before one can determine the nature of the confining interaction (and then only in the region directly sampled by the bound states).

TABLE II. Comparison of the exact ground-state energies for the Coulomb-plus-linear potential  $V = -ar^{-1} + br$  with the parameters of Ref. 26 with the first-order energies calculated by minimizing the SVZ exponential moments function  $R_l^{(1)}$ , Eq. (74). The masses of the charm and bottom quarks are  $m_c = 1.35$  GeV and  $m_b = 4.77$  GeV. The last two columns give the results obtained for  $b$ -quarkonium when the potential is modified so that the first-order  $1S$  and  $1P$  charmonium energies are correct.

State	$a=0.49, b=0.17 \text{ GeV}^2$			$a=0.665, b=0.146 \text{ GeV}^2$	
	$E_{1l,\text{exact}}$ (MeV)	$E_{1l}^{(1)}$ (MeV)	Error (MeV)	$E_{1l}^{(1)}$ (MeV)	Error (MeV)
<b>Charmonium</b>					
1S	364	508	+ 144	364	Fitted
1P	772	914	+ 142	772	Fitted
1D	1060	1221	+ 161	1063	+ 3
1F	1305	1487	+ 182	1314	+ 9
<b><math>b</math>-quarkonium</b>					
1S	-98	106	+ 204	-94	+ 4
1P	349	479	+ 130	343	-6
1D	585	714	+ 129	581	-4
1F	769	905	+ 136	767	-2

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<sup>19</sup>We choose to work with the perturbation expansion of  $-\ln K$  for the same reason that one works with the expansion of the logarithm of the partition function (the free energy) in statistical mechanics (the problems are equivalent, with  $\tau \leftrightarrow 1/kT$ ):  $K(0,0,-i\tau)$  is essentially exponential, and the (cumulant) expansion of  $\ln K$  in  $K = \exp(\ln K)$  gives an efficient approximation of high-order terms in  $K$ . See, for example, L. E. Reichl, *A Modern Course in Statistical Physics* (University of Texas Press, Austin, 1980). In the cases we have checked, the alternative procedure of expanding  $K$  in perturbation series and equating  $R$  to the (unexpanded) ratio  $-K'/K$  is significantly inferior to that used here. [The equivalent of the alternative procedure was used, for example, by RRY (Ref. 2) in their power-moments calculations.]

<sup>20</sup> $R^{(1)}(\tau)$  is positive and decreasing [ $(dR^{(1)}/d\tau) < 0$ ] for  $\tau$  sufficiently small for any potential less singular than  $r^{-2}$  at the origin, and is of course bounded below by  $E_{1s}$ .  $R^{(1)}(\tau)$  must therefore have a finite minimum value on  $(0, \infty]$  for any such potential with a spectrum bounded from below, in particular, for any confining potential.

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<sup>27</sup>The coefficients  $f_n$  in the expansion

$$\mathcal{A}(x) = \frac{3}{2x} - \left[ 1 + \frac{\nu}{2} \right] \sum_{n=1}^{\infty} n f_n x^{n-1+\nu/2}$$

are easily calculated recursively from the coefficients  $g_n$  which appear in the expansion

$$(4\pi\tau/m_q)^{3/2} K(0,0,-i\tau) = 1 + \sum_{n=1}^{\infty} g_n x^{n+\nu/2}$$

by using the formulas

$$f_1 = g_1, \\ f_{n+1} = g_{n+1} - \frac{1}{n+1} \sum_{i=0}^{n-1} (i+1) g_{n-i} f_{i+1}, \quad n \geq 1.$$



See J. B. Whinton, University of Wisconsin dissertation, 1982 (unpublished), Appendix H.

<sup>28</sup>The existence of the inflection points is associated with nearby complex-conjugate zeros in  $d\mathcal{R}_0^{(2)}/dx$ . In all the cases we have checked, the value of  $x$  at the inflection point is essentially equal to the real part of  $x$  at the complex zero. The inflection-point criterion therefore picks out the "complex minimum" of  $\mathcal{R}_0^{(2)}$  and generalizes the usual minimum criterion.

<sup>29</sup>George A. Baker, *Essentials of Padé Approximants* (Academic, New York, 1975).

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$$V(r) = -\frac{4\alpha_s}{3r} + \frac{8}{5} \left\{ \left[ \left[ \frac{3\alpha_s}{2r} \right]^2 + \frac{5}{32} \phi_1 r^2 \right]^{1/2} - \frac{3\alpha_s}{2r} \right\}.$$

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