Moment-problem formulation of a minimax quantization procedure

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The eigenvalue moment method (EMM) is a general theory for generating converging lower and upper bounds to the discrete, low-lying spectrum of Schrödinger Hamiltonians. Recently, Handy, Giraud, and Bessis [Phys. Rev. A **44**, 1505 (1991)] developed a dynamical systems EMM formulation through the discovery of a fundamental convex function, $F_E[u]=\mathrm{Min}_{\sigma=0,1}\langle V^{(\sigma,E)}[u]|\mathcal{M}^{(\sigma,E)}[u]|V^{(\sigma,E)}[u]\rangle$. By incorporating this within the c-shift EMM theory of Handy and Lee [J. Phys. A **24**, 1565 (1991)], there results an alternative quantization procedure involving the function $\mathcal{V}(E)=\mathrm{Max}_u\mathrm{Min}_{\sigma=0,1}\langle V^{(\sigma,E,S)}[u]|S_\sigma^{-1}\mathcal{M}^{(\sigma,E)}[u]S_\sigma^{-1}|V^{(\sigma,E,S)}\rangle$, whose local maxima converge to the discrete energy states of the system. We discuss the relevant theory and present several examples.

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I. INTRODUCTION

The development of effective theoretical and computational quantum energy bonding methods has been an ongoing problem for many years. This has been motivated, in part, by the need to solve difficult singular problems whose analysis through conventional methods has resulted in significantly varying predictions. One of the most well known is the quadratic Zeeman effect for superstrong magnetic-field strengths, amply reviewed in the work of Le Guillou and Zinn-Justin [1]. The obtainment of tight bounds through Handy *et al.*'s eigenvalue moment method (EMM) [2] defined a linear optimization [3] approach for confirming the accuracy of their results through the generation of converging lower and upper bounds to the ground-state binding energy. Subsequent investigations by Fonte *et al.* [4] and Falsaperla and Fonte [5] utilized basis-dependent, nonlinear variational methods based on the classic work of Kato [6], achieving results consistent with those of EMM theory.

In general, the development of energy bounding methods is a difficult problem. This has been particularly the case with respect to the generation of converging lower bounds for the ground-state energy of quantum systems. Indeed, many of the traditionally important works readily acknowledge this and limit their applicability to semibounded Hamiltonians, or equivalently those with a non-negative potential, $V\geq 0$. Some of the more notable of these approaches are Löwdin's inner projection method [7], Cizek and Vrscay's renormalized inner projection method [8], and the Green's-function based analysis reviewed by Bertlmann [9]. By way of contrast, one unique advantage the EMM approach enjoys over these methods is that there is no semiboundedness restriction on the Hamiltonian. It is applicable even for unbounded Hamiltonians. The aforementioned quadratic Zeeman effect is a case in point.

Another important class of bounding methods is those combining large order perturbation theory with important mathematical theorems on the Stieltjes nature of the underlying Rayleigh-Schrödinger perturbation series. Simon [10] established the fundamental result that the underlying perturbation series for the quartic anharmonic potential is Stieltjes. This led to the generation of lower and upper bounds to the ground-state energy. Related works by Bender and Wu [11] showed that for the quartic and sextic anharmonic oscillators, the Carleman uniqueness conditions were satisfied permitting the generation of converging lower and upper bounds to the physical ground-state energy. The octic anharmonic oscillator does not fall into this category and cannot be tightly bounded through Stieltjes based methods [12]. Accordingly, Vinette and Cizek [13] utilized a renormalized inner projection method to generate converging bounds. The EMM approach [2,14] is a nonperturbative method that automatically guarantees uniqueness leading to the systematic generation of converging lower and upper bounds. The application to the octic anharmonic oscillator is immediate [15,16] and duplicates the results of Vinette and Cizek.

The EMM approach entails a subtle projection method philosophy designed to take advantage of the unique positivity structure (for bosonic ground states) and asymptotic features of physical wave function (bound-state) configurations [2,14]. It does this through the transformation of the configuration-space problem into a moment-problem formulation (Shohat and Tamarkin [17]). For excited states, the addition of a constant background "shift" term, combined with an appropriate regulating multiplicative function factor, leads to an effective bounding method as well [18].

Other moment based quantization methods have been developed over the last two decades: Killingbeck [19], Richardson and Blankenbecler [20], and Killingbeck,

Jones, and Thompson [21]. However, none of these is a true moment-problem formulation. These alternate approaches do not yield bounds, and may require delicate asymptotic estimates for the moments which can be difficult to obtain for multidimensional problems. Nevertheless, in those cases of applicability, the results have been impressive.

In addition to the fundamental theoretical and computational advantages afforded by the EMM approach, as outlined briefly above, its inherent structure has led to some other important developments: (1) EMM marks the first significant use of linear programming optimization methods [3] in quantum physics [2]. (2) Its recent reformulation from a dynamical systems' perspective [22] highlights the important role convexity plays in quantum mathematical physics. (3) EMM was specifically designed to tackle singular perturbation type problems, and therefore complements ordinary (including large order) perturbation theory. This is because it is a Fourier space based method in which the power moments are essentially the Taylor expansion coefficients of the wave function around the origin in momentum space. Our extensive numerical experience reveals that with very little sophistication (beyond that ingrained in the method itself) EMM is very effective, particularly for strong (large) coupling regimes. As evidence of this, the direct application of EMM to the quadratic Zeeman effect [2] yielded remarkably consistent results with those afforded through Le Guillou and Zinn-Justin's order dependent conformal analysis [1]. (4) Finally, EMM theory is intrinsically a multiscale approach [23]. It is a global theory proceeding from large spatial scales down to smaller scales.

Although the major focus of the preceding remarks has been with respect to the generation of eigenenergy bounds, it is also possible to use EMM as an estimation method, thereby avoiding the computationally expensive process of generating bounds. This can be very important, given the other significant aspects of the method. This is the principal objective of this work. Based on two earlier works [18,22], we will be able to define an alternative functional expression (the *volcano function*) whose local maxima along the energy axis correspond to arbitrarily accurate estimates for the low-lying bound-state spectrum. This approach defines a potentially significant eigenvalue estimation method applicable to multidimensional problems, although demonstrated here through two pedagogic one-dimensional cases. The first of these is the simple harmonic-oscillator problem. The second corresponds to the well studied rational fraction potential problem $x^2+\lambda[x^2/(1+gx^2)]$ reviewed by Hodgson [24].

II. OVERVIEW OF EMM

As indicated in the Introduction, EMM is a general theory for generating converging lower and upper bounds to the low-lying discrete spectrum of arbitrary Schrödinger Hamiltonians. It has been very successful in the analysis of singular systems, yielding tight bounds to the ground-state eigenvalue. Some significant applications have been to the following: the quadratic Zeeman effect [2], which yielded some of the first rigorous and tight bounds to this important problem; the analysis [25] of the potential $x^2+\lambda[x^2/(1+gx^2)]$, which refuted the accuracy of a previous Hellmann-Feynman hypervirial analysis by Lai and Lin [26], subsequently reconfirmed by Hodgson [24]; analysis of the double-well quartic anharmonic oscillator [27], which yielded exceptionally tight bounds and corrected some slight inaccuracies in the results of de Saavedra and Buendia [28,29]; Handy *et al.*'s [30] comprehensive analysis of various one-dimensional problems appearing in the literature [31–37].

The basic EMM philosophy involves transforming a given Schrödinger system into a moment-problem formulation, followed by the imposition of positivity constraints on the moments, as dictated by the positivity structure of the associated wave function, $\Psi(x)$ [2,5]. This process defines constraints on the energy. The original formulations by Handy and co-workers focused primarily on the bosonic ground state because of the well-known property that the multidimensional bosonic ground-state wave function must be of uniform signature and can thus be taken to be positive, $\Psi(x)>0$ [38]. Subsequent studies yielded a more comprehensive theory applicable to arbitrary excited states, culminating in the *c*-shift EMM Formulation by Handy and Lee [18].

The latter work involves adding a sufficiently positive constant c to the wave function $\Psi(x)$ followed by the multiplication with respect to a suitable positive regulating function, $R(x)$: $[\Psi(x)+c]R(x)=\Phi(x)$. The basic EMM theory is then developed within the $\Phi(x)$ representation. One does not know *a priori* the minimum positive c value to take ($c>c_{\min}>0$), for a given excited state, which will make the corresponding $\Phi(x)$ positive. However, this can be empirically determined [18].

Most of the aforementioned works relied heavily on the use of linear programming methods [3] to solve the positivity constraint relations on the moments [2]. For large dimensioned systems, this basic approach (involving the "cutting method" [2]) is potentially inefficient (because of large computer memory allocation requirements). Numerical experiments revealed that there was an inherent dynamical systems' behavior to the linear programming based methodology. Handy, Giraud, and Bessis [22] discovered an important convex function $F_E[u]$ central to the EMM theory, leading to a potentially more efficient Newton-iteration EMM reformulation. This approach is referred to as the dynamical system EMM formulation or DS-EMM.

We shall refer to $F_E[u]$ as the *volcano function,* for aesthetic reasons motivated by the case of the sextic anharmonic oscillator (graphically illustrated in this work). The volcano function is parametrized by the energy, E, and is convex only with respect to its *missing moment,* u, dependence. Generally, it is a continuous, piecewise differentiable function of u. The DS-EMM reformulation involves almost no linear programming, and is in principle superior to any previous EMM algorithms.

From the volcano-function perspective, quantization is achieved by determining the (approximate) energy values where the volcano function emerges from $(E_i^{(-)})$, and submerges under $(E_i^{(+)})$, the missing moment space hyperplane(sea). These consecutive energy values define the lower and upper bounds, respectively, to the desired

eigenenergy ($E_i^{(-)} \leq E_i \leq E_i^{(+)}$). In other words, for each energy parameter value lying within these bounds ($E_i^{(-)} \leq E \leq E_i^{(+)}$) the volcano function will take on non-negative values on a convex subset, $U_s[E]$, of the missing moment space: $F_E[u] \geq 0$ for $u \in U_s[E]$ and $E \in [E_i^{(-)}, E_i^{(+)}]$. A suggestive picture is given in Fig. 1 corresponding to the case of the sextic anharmonic oscillator. This example is solely for the ground-state case ($i=0$).

If the DS-EMM formulation is applied within the original EMM framework, then only the ground-state energy E_0 is obtainable. We shall refer to this as the *ground-state volcano-function formulation.* If instead, DS-EMM is applied to the c-shift EMM formulation (explicitly working with a fixed and sufficiently positive c background term), then the corresponding volcano function will repeatedly emerge and submerge from the missing moment sea, resulting in the quantization of the appropriate ground and excited state E_i's [that is, for all those bound states for which the chosen c value yields non-negative $\Phi_i(x)$ configurations, $\Phi_i(x) \geq 0$]. We will refer to this formulation by DS-EMM/C. The distinction between both approaches will become clear in the subsequent analysis.

Clearly, in order to determine the aforementioned eigenenergy bounds, one need not refer to the entire volcano function, just to the E-dependent expression $\mathcal{V}(E) = \mathrm{Max}_u F_E[u]$. We shall also refer to $\mathcal{V}(E)$ as the volcano function.

An interesting and important question is: within the ground-state volcano-function formulation what happens to the volcano function for arbitrary values of the energy parameter beyond those corresponding to the ground-state energy? Numerical experiments suggest that the function $\mathcal{V}(E)$ will oscillate. That is, it will manifest multiple local maxima, each approximating one of the

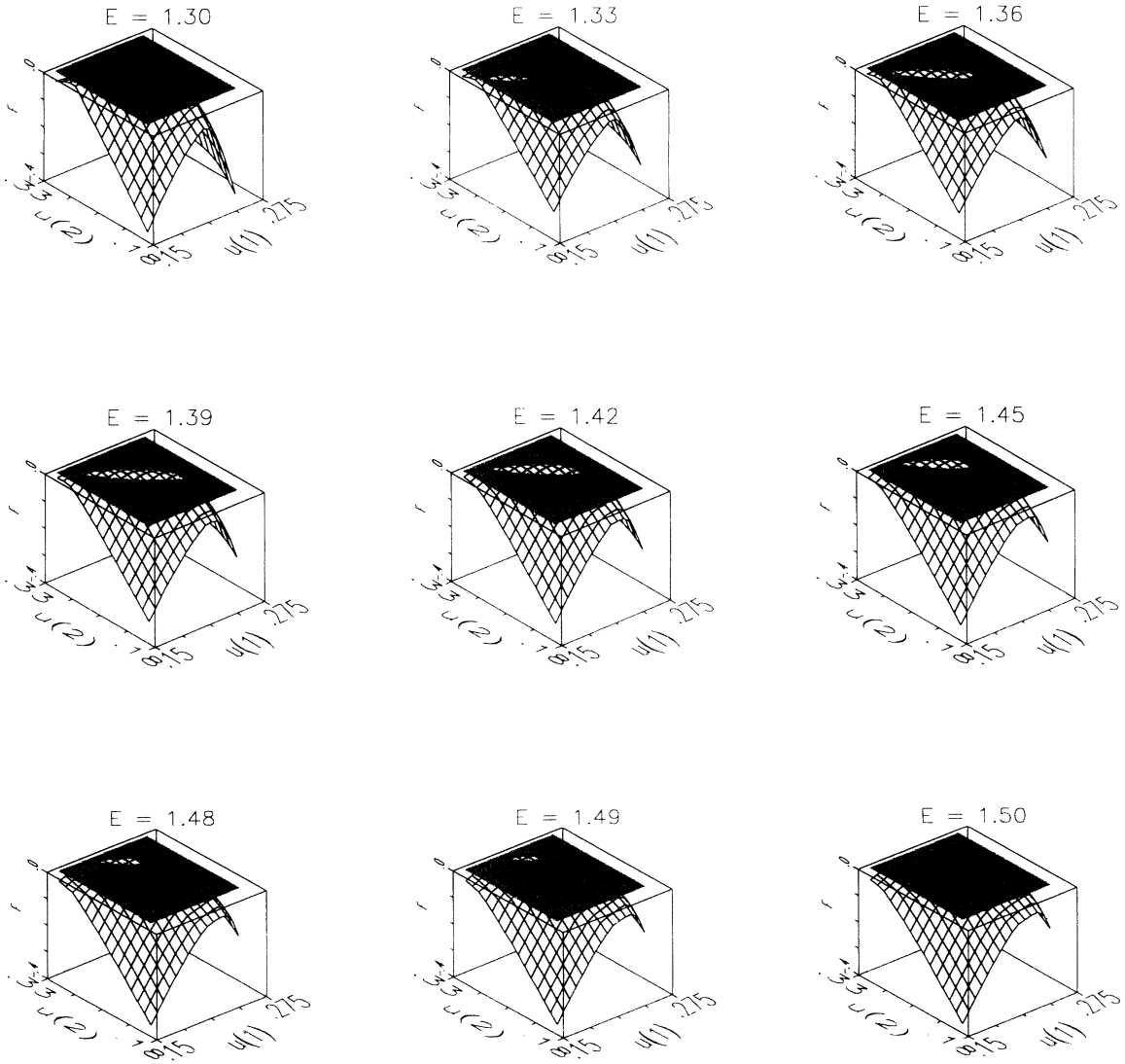

FIG. 1. Side view of the emergence and submergence of the volcano function for the sextic oscillator potential problem ($m = g = 1$). The maximum moment order $P_{\max}$ is 6.

discrete energy states. We cannot prove this directly within the ground-state volcano-function formulation; however, we can define an equivalent but alternate volcano-function representation in which the above can be proven. Essentially, we will show that by a clever transformation we can effectively "subtract" out the background c term, as defined previously, within the DS-EMM/C representation.

Since all of the necessary formalism is fully developed in the cited references, we shall only outline the necessary results in the next section.

III. A GENERIC CASE: THE SEXTIC ANHARMONIC OSCILLATOR

Consider the sextic anharmonic oscillator problem corresponding to

$$-\frac{d^2\Psi}{dx^2}+[mx^2+gx^6]\Psi(x)=E\Psi(x)\ . \tag{3.1}$$

Define the Hamburger moments $\mu(p)=\int_{-\infty}^{+\infty}x^p\Psi(x)dx$. Through a simple integration by parts, we can transform Eq. (3.1) into a Hamburger moment equation:

$$\mu(p+6)=g^{-1}[-m\mu(p+2)+E\mu(p) +p(p-1)\mu(p-2)]\ . \tag{3.2}$$

For simplicity, we can limit the analysis to the even parity states. Thus $\mu(\text{odd})=0$. Accordingly, one can work with the even order Hamburger moments $\mu(2p)\equiv u(p)$, where the latter are Stieltjes moments of the configuration $y^{-1/2}\Psi(y^{1/2})$, as defined by $u(p)=\int_0^{+\infty}y^{p-1/2}\Psi(y^{1/2})dy$. In terms of the Stieltjes moments, the corresponding equation becomes

$$u(p+3)=g^{-1}[-mu(p+1)+Eu(p) +2p(2p-)u(p-1)]\ . \tag{3.3}$$

The above equation defines a homogeneous, linear, (effectively) third order finite difference equation where the moments $u(0)$, $u(1)$, and $u(2)$ must be specified before all the other moments can be generated. These initialization variables are referred to as *missing moments.* The homogeneous character requires the imposition of some appropriate normalization condition. We generally choose the sum of the missing moments to be unity, $u(0)+u(1)+u(2)=1$. This in turn leads to there being only two unconstrained missing moments, $u(1)$ and $u(2)$. We can then symbolize the linear dependence on the unconstrained missing moments by the expression

$$u(p)=\sum_{l=0}^{2}\hat{M}_E(p,l)\hat{u}(l)\ , \tag{3.4}$$

where $\hat{u}(0)\equiv 1$ and $\hat{u}(i\neq 0)\equiv u(i)$. The energy, E, dependent $\hat{M}_E(p,l)$ coefficients can be easily generated numerically. We shall refer to $u(1)$ and $u(2)$ by u_1 and u_2, respectively.

In terms of the DS-EMM theory [22], quantization of the ground-state energy, E_0, proceeds as follows. Consider the missing-moment-dependent, energy-parametrized volcano $F_E[u_1,u_2]$ defined by [$\mathbf{u}$ denotes the vector (u_1,u_2)]:

$$F_E[\mathbf{u}]\equiv \mathrm{Min}_{\sigma=0,1}\left[\sum_{i_1=0}^{I}\sum_{i_2=0}^{I}V_{i_1}^{(\sigma,E)}[\mathbf{u}]\left[\sum_{l=0}^{2}\hat{M}_E(\sigma+i_1+i_2,l)\hat{u}(l)\right]V_{i_2}^{(\sigma,E)}[\mathbf{u}]\right]\ , \tag{3.5}$$

where the vector $V^{(\sigma,E)}$ (which is implicitly dependent on σ, E, and $\mathbf{u}$) denotes (throughout this work) the normalized eigenvector for the lowest eigenvalue of the associated Hankel matrix

$$\mathcal{M}_{i_1,i_2}^{(\sigma,E)}[\mathbf{u}]=\begin{cases}u(\sigma+i_1+i_2) & \text{or}\\ \displaystyle\sum_{l=0}^{2}\hat{M}_E(\sigma+i_1+i_2,l)\hat{u}(l)\ .\end{cases} \tag{3.6}$$

Alternatively, we will symbolize Eq. (3.5) by

$$F_E[\mathbf{u}]\equiv \mathrm{Min}_{\sigma=0,1}\langle V^{(\sigma,E)}[\mathbf{u}]|\mathcal{M}^{(\sigma,E)}[\mathbf{u}]|V^{(\sigma,E)}[\mathbf{u}]\rangle\ , \tag{3.7a}$$

or

$$F_E[\mathbf{u}]\equiv \mathrm{Min}_{\sigma=0,1}\lambda^{(\sigma,E)}[\mathbf{u}]\ , \tag{3.7b}$$

where $\lambda^{(\sigma,E)}[\mathbf{u}]$ is the smallest eigenvalue of the associated Hankel matrix.

It has been proven elsewhere that $F_E[\mathbf{u}]$ is a convex function with respect to its u dependence [22]. As such, it can only have, at most, one extremum value, a maximum. We denote this by $\mathcal{V}(E)$. Either of these functions is referred to as the *volcano* function.

Up to order I [refer to E.q (3.5)], the E interval on which $V(E)\geq 0$, defines the "feasible" energy interval $[E_0^{(-)},E_0^{(+)}]$ within which the physical ground-state eigenvalue E_0 lies: $E_0^{(-)}\leq E_0\leq E_0^{(+)}$. As more moments are used ($I\rightarrow\infty$) the lower and upper bounds converge to the true physical value. In other words, the E interval on which the volcano function is positive contracts to a point.

In Fig. 1 we show the behavior of the volcano function $F_E[\mathbf{u}]$ for various E values. The true ground-state energy is $E_0=1.4356$ [14]. The series of illustrations shows the volcano function emerging and submerging relative to the missing moment space plane (sea).

IV. OSCILLATIONS OF THE VOLCANO FUNCTION

Let us consider the c-shift formulation of Handy and Lee [18], in which the objective is to extend the EMM philosophy to excited states. In general, excited multidimensional bosonic wave functions, $\Psi(x)$, have no definite

signature. As such, the basic EMM formulation, as outlined in Sec. III, cannot be applied directly. Instead, by adding a sufficiently positive constant c together with the multiplication by a suitable positive regulating function $R(x)$ (as determined through a zeroth-order JWKB analysis) one can work within a new configuration space, $\Phi(x)=[\Psi(x)+c]R(x)$, where the desired excited states are uniquely positive and asymptotically bounded (relative to all the infinitely many unphysical solutions of the associated Schrödinger system). This is critical if the EMM theory is to work. In general, the determination of the appropriate c value is done empirically [18]. For the sextic anharmonic oscillator case, one may take $R(x)=\exp(-\alpha x^2)$, for arbitrary positive α.

In the work by Handy and Lee, a moment equation is derived for the $\Phi(x)$ configuration. We will depart, slightly, from their formalism and instead focus on the moments of $\Omega(x)=\Psi(x)R(x)$ and $cR(x)$, separately. For simplicity, we limit our analysis to the symmetric states only. Furthermore, as was done in the preceding section, we will adopt the Stieltjes moment representation [refer to the discussion pertaining to Eq. (3.3)]. The Stieltjes moments of $\Omega(x)$ and $R(x)$ are denoted by $w(p)$ and $v(p)$, respectively. A Stieltjes moment equation ensues for $\Omega(x)$:

$$w(p+3)=g^{-1}\{[4\alpha^2-m]w(p+1)-[8\alpha p+2\alpha-E]w(p)+2p(2p-1)w(p-1)\}\ , \tag{4.1}$$

for $p\geq 0$.

We may impose an arbitrary normalization, such as $w(0)+w(1)+w(2)=1$, and proceed to eliminate $w(0)$. Note that $w(0)$, $w(1)$, and $w(2)$ may become nonpositive, for the physical solutions. However, even for such a possibility, it is highly unlikely that the adopted normalization will be invalid [i.e., $w(0)+w(1)+w(2)=0$]. If the adopted normalization is inappropriate for the desired quantum state(s), then one must choose some other normalization constraint. In any case, a wrong choice of normalization will result in the associated quantum state(s) being projected out. That is, only those energies which are consistent with the adopted normalization will be obtainable. An important observation is that since no linear programming is required within the present "volcano-function" formulation, one does not need to insist that the missing moments be positive, and through the normalization, limited to a bounded region. Note also that one must be careful to choose a regulating function $R(x)$ which is not orthogonal to the desired excited states.

Let $u(p)$ denote the corresponding Stieltjes moments for the $\Phi(x)$ configuration. We may then write $[u(p)=w(p)+cv(p)]$,

$$u(p)=\sum_{l=0}^{2}\hat{M}_E(p,l)\hat{w}(l)+cv(p)\ , \tag{4.2}$$

where the coefficients $\hat{M}_E(p,l)$ are readily obtainable.

For a fixed, and sufficiently positive, c value we can proceed to quantize all the excited states whose associated Φ configurations are positive. That is, consider the volcano-function expression for the u moments as functions of w [note, $\mathbf{w}=(w(1),w(2))$]:

$$F_{E,c}[\mathbf{w}]\equiv \mathrm{Min}_{\sigma=0,1}\langle V^{(c,\sigma,E)}[\mathbf{w}]|(\mathcal{M}^{(\sigma,E)}[\mathbf{w}]+c\mathcal{M}^{(\sigma)}[v])|V^{(c,\sigma,E)}[\mathbf{w}]\rangle\ , \tag{4.3}$$

where the $\mathcal{M}$ Hankel matrices are defined as before with respect to their respective moments [refer to Eq. (3.6)]. We have explicitly indicated which expressions depend on the energy parameter, E. Through the w-moment equation and the adopted normalization condition, the Hankel matrix for the $w(p)$ Stieltjes moments, $\mathcal{M}^{(\sigma,E)}[\mathbf{w}]$, depends on the energy and the unconstrained missing moments [$w(1)$ and $w(2)$]; while the Hankel matrix $\mathcal{M}^{(\sigma)}[v]$ is independent of E. As indicated before, $V^{(c,\sigma,E)}[\mathbf{w}]$ is the normalized eigenvector for the smallest eigenvalue of the full Hankel matrix appearing within the Dirac bra-ket, $\mathcal{M}^{(\sigma,E)}[\mathbf{w}]+c\mathcal{M}^{(\sigma)}[w]$.

The associated volcano function, $\mathcal{V}_c(E)=\mathrm{Max}_w F_{E,c}[\mathbf{w}]$, will generally be non-negative over several E intervals $\{[E_i^{(-)},E_i^{(+)}]\}$, and negative elsewhere. Each of these contains the corresponding (ground or excited state) energy eigenvalue, E_i. The end points of a given interval will define lower and upper bounds to the respective E_i: $E_i^{(-)}\leq E_i\leq E_i^{(+)}$. So long as c is held fixed and sufficiently positive, as the order of the calculation increases these energy intervals will become smaller, the bounds becoming tighter. In other words, $\mathcal{V}_c(E)$ undergoes continuous oscillations between negative and positive values, which become more peaked as the other of the calculation increases. Observe that because of the E and w dependence of the

$$\langle V^{(c,\sigma,E)}[\mathbf{w}]|c\mathcal{M}^{(\sigma)}[v]|V^{(c,\sigma,E)}[\mathbf{w}]\rangle$$

term in Eq. (4.3), one cannot trivially subtract out the c dependence from $\mathcal{V}_c(E)$. That is, there is no guarantee that $\mathcal{V}_{c=0}(E)$ will oscillate in a manner similar to $\mathcal{V}_c(E)$. Nevertheless, we can effectively do this as follows.

The Hankel matrix $\mathcal{M}^{(\sigma)}_{i_1,i_2}[v]=v(\sigma+i_1+i_2)$ in Eq. (4.3) is a symmetric and positive definite matrix because it involves the moments of a positive function, $R(x)$. Accordingly, one can define its square root, S_σ, or $\mathcal{M}^{(\sigma)}[v]=S_\sigma^2[v]$. The square root matrix and its inverse (which must exist because of $\mathcal{M}^{(\sigma)}[v]$'s positive definiteness) can be taken to be positive and symmetric as well. We may rewrite the Hankel matrix appearing in Eq. (4.3) as

$$\mathcal{M}^{(\sigma,E)}[\mathbf{w}]+c\mathcal{M}^{(\sigma)}[\mathbf{v}]=S_\sigma[v](S_\sigma^{-1}[v]\mathcal{M}^{(\sigma,E)}[\mathbf{w}]S_\sigma^{-1}[v]+c\underline{1})S_\sigma[v]\ . \tag{4.4}$$

From the Appendix, it follows that the volcano functions for the matrices $\mathcal{M}^{(\sigma,E)}[\mathbf{w}]+c\mathcal{M}^{(\sigma)}[\mathbf{v}]$ and $S_\sigma^{-1}[v]\mathcal{M}^{(\sigma,E)}[\mathbf{w}]S_\sigma^{-1}[v]+c\underline{1}$ must have the same signature and therefore lead to the same quantization results. Let us denote the respective volcano functions by $\mathcal{V}_c[E]=\mathrm{Max}_{\mathbf{w}}\{F_{E;c}[\mathbf{w}]\}$ and $\mathcal{V}_c^{(S)}[E]=\mathrm{Max}_{\mathbf{w}}\{F_{E;c}^{(S)}[\mathbf{w}]\}$ where

$$F_{E;c}[\mathbf{w}]=\mathrm{Min}_{\sigma=0,1}\{\langle V^{(c,\sigma,E)}[\mathbf{w}]|(\mathcal{M}^{(\sigma,E)}[\mathbf{w}]+c\mathcal{M}^{(\sigma)}[v])|V^{(c,\sigma,E)}[\mathbf{w}]\rangle\}\ , \tag{4.5a}$$

and

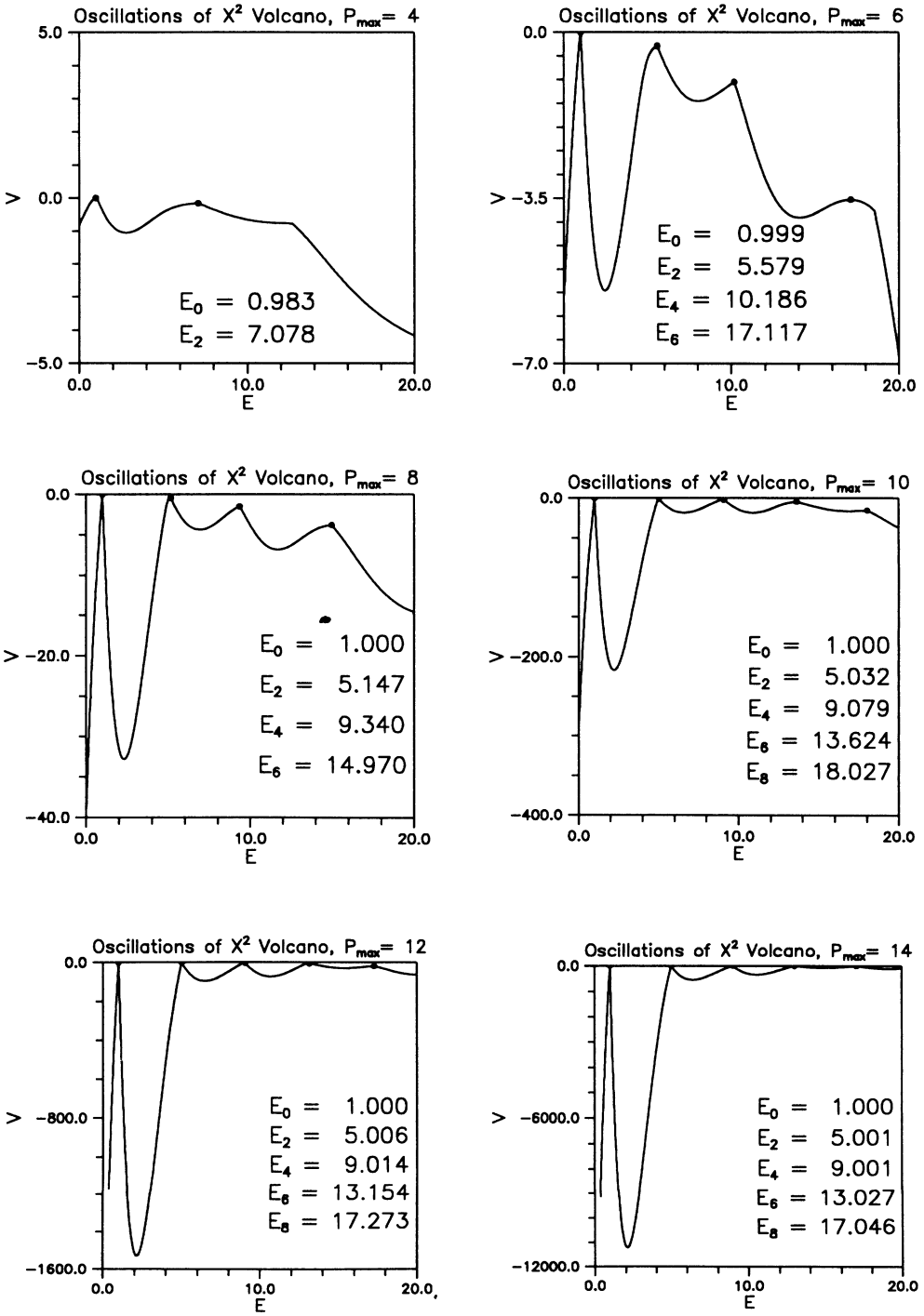

FIG. 2. Oscillations of the volcano function for the harmonic-oscillator potential. Exact symmetric state energies are 1, 5, 9, 13, 17, etc.

$$F^{(S)}_{E;c}[\mathbf{w}]=\mathrm{Min}_{\sigma=0,1}\{\langle V^{(\sigma,E,S)}[\mathbf{w}]|(S_\sigma^{-1}[v]\mathcal{M}^{(\sigma,E)}[\mathbf{w}]S_\sigma^{-1}[v]+c\underline{1})|V^{(\sigma,E,S)}[\mathbf{w}]\rangle\}\ ,$$

or (4.5b)

$$F^{(S)}_{E;c}[\mathbf{w}]=\mathrm{Min}_{\sigma=0,1}\{\langle V^{(\sigma,E,S)}[\mathbf{w}]|(S_\sigma^{-1}[v]\mathcal{M}^{(\sigma,E)}[\mathbf{w}]S_\sigma^{-1}[v])|V^{(\sigma,E,S)}[\mathbf{w}]\rangle\}+c\ ,$$

(because $\langle V^{(\sigma,E,S)}[\mathbf{w}]|V^{(\sigma,E,S)}[\mathbf{w}]\rangle\equiv 1$). The signatures of $\mathcal{V}_c[E]$ and $\mathcal{V}_c^{(S)}[E]$ must be identical, because the same is true for $F_{E;c}[\mathbf{w}]$ and $F^{(S)}_{E;c}[\mathbf{w}]$ (see Appendix). An important result is that

$$\mathcal{V}_c^{(S)}[E]=\mathcal{V}_0^{(S)}[E]+c\ . \tag{4.6}$$

Let us now focus on the significance of Eq. (4.6). Through EMM theory, we know that for a sufficiently

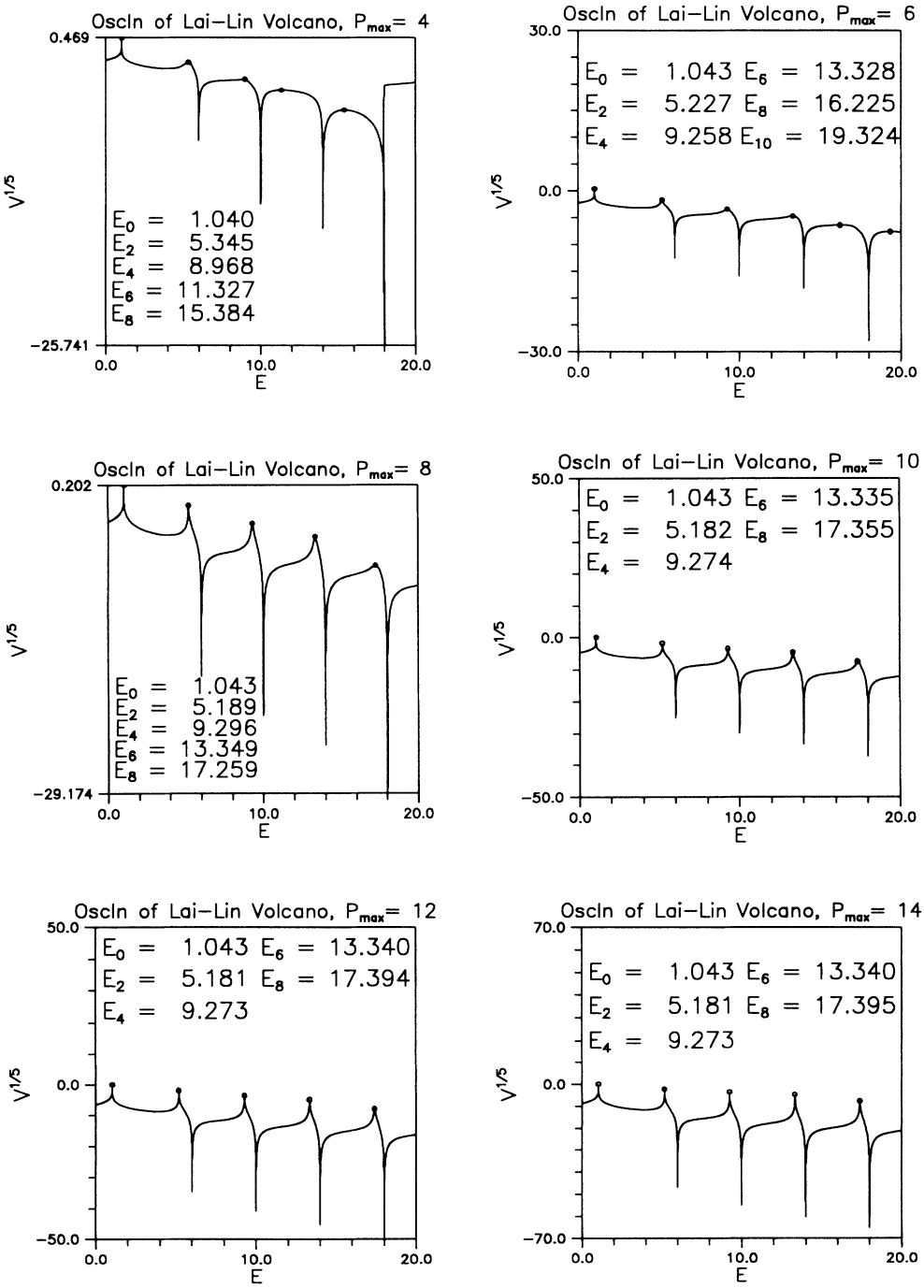

FIG. 3. Oscillations of the volcano function for the Lai-Lin rational fraction potential ($g=\lambda=0.1$). Results of Roy, Roychoudhury, and Roy [35] for the first two symmetric states are 1.043 140 and 5.181 319.

large and positive c the volcano function $\mathcal{V}_c^{(S)}[E]$ will be positive over several E intervals, and negative elsewhere. As the order of the calculation increases, while keeping c fixed, these E intervals become smaller, generating through their end points converging lower and upper bounds to the corresponding discrete state energies of the system. A plot of $\mathcal{V}_c^{(S)}[E]$ will reveal this oscillatory behavior. Clearly, a simple subtraction of the c constant will not affect the basic form of these oscillations, which become highly peaked as the order of the calculation increases. In other words, we can use the local maxima of $\mathcal{V}_0^{(S)}[E]$ to approximate the discrete energies.

V. NUMERICAL EXAMPLES

In order to demonstrate the consequences of the preceding analysis, we will examine two problems, each corresponding to zero-missing moments. The first is the harmonic oscillator, the other is the rational fraction potential $x^2+\lambda[x^2/(1+gx^2)]$, well documented in the literature [24–26]. In each case, we will limit the analysis to the symmetric states only, for convenience.

Consider the harmonic-oscillator problem

$$-\frac{d^2\Psi}{dx^2}+mx^2\Psi(x)=E\Psi(x)\ . \tag{5.1}$$

Performing the transformation $\Phi(x)=\Psi(x)\exp(-\alpha x^2)$, where according to Handy and Lee one must impose the conditions $0\le\alpha\le\sqrt{m}\ /2$, the Φ-Stieltjes moment equation ensues:

$$w(p+1)=\frac{\{[E-8\alpha p-2\alpha]w(p)+2p(2p-1)w(p-1)\}}{m-4\alpha^2}, \tag{5.2}$$

with normalization $w(0)=1$. The regulating function $\exp(-\alpha x^2)$ has Stieltjes moments $v(p)$ satisfying

$$v(p+1)=(2\alpha)^{-1}(2p+1)v(p)\ , \tag{5.3}$$

with $v(0)=\sqrt{\pi/\alpha}$. One can now readily evaluate the square roots of the Hankel matrices $v(i+j)$ and $v(1+i+j)$. In Fig. 2 we show the behavior of the volcano function, as a function of the energy ($\alpha=\frac{1}{4}$). The reader will note the increased peaked nature of the local extrema, as the order of the calculation increases ($P_{\max}\equiv$maximum order of moments used). The exact symmetric state eigenvalues ($m=1$) are 1, 5, 9, 13, etc.

Consider now the rational fraction potential problem

$$-\frac{d^2\Psi}{dx^2}+\left[x^2+\lambda\frac{x^2}{(1+gx^2)}\right]\Psi(x)=E\Psi(x)\ . \tag{5.4}$$

We may use the regulator function $\exp(-x^2/2)$. The corresponding Φ-moment equation is

$$w(p+1)=\frac{\{1+E+[2g(p+1)-2](2p+1)\}w(p)+2p(2p-1)w(p-1)}{2g(2p+3)+\lambda-g(1+E)}\ . \tag{5.5}$$

The volcano-function analysis proceeds as in the previous case. The graphical results are given in Fig. 3. For the case depicted ($g=\lambda=0.1$) the low-lying, symmetric state energies are as given in the figures. The recent work of Roy, Roychoudhury, and Roy [35] establishes the approximate values for the first two symmetric state energies: 1.043 140 and 5.181 319. The results obtained through the volcano-function approach, as reflected in Fig. 3, give the eigenenergy estimates up to the third decimal place (for the approximate extremal points). A finer energy-axis partitioning would be required in order to compare with the results of Roy, Roychoudhury, and Roy.

VI. CONCLUDING REMARKS

We have shown how the DS-EMM formulation, in the context of the c-shift EMM formalism, leads to an oscillating function of the energy whose local maxima approximate the discrete energies of the system, arbitrarily well. Although the preceding analysis required the square root matrix, S, of the positive definite Hankel matrix $\mathcal{M}$, the numerical costs of this procedure can be significantly reduced by working instead with the Cholevsky decomposition of $\mathcal{M}$ [39]. Specifically, we may write $\mathcal{M}=\mathcal{C}\mathcal{C}^\dagger$ (where $\mathcal{C}=\mathcal{L}\mathcal{D}^{1/2}$, corresponding to the LU decomposition $\mathcal{M}=\mathcal{L}\mathcal{D}\mathcal{L}^\dagger$). One can then work with the volcano function corresponding to the matrix $\mathcal{C}^{-1}\mathcal{M}[\mathbf{w}]\mathcal{C}^{\dagger-1}$ [in a manner analogous to Eq. (4.4)].

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APPENDIX

Consider an arbitrary symmetric matrix $\mathcal{M}$ and a positive definite symmetric matrix, S. Let V and V_S denote the normalized eigenvectors of $\mathcal{M}$ and $\mathcal{M}_S=S^{-1}\mathcal{M}S^{-1}$, corresponding to the smallest eigenvalues, λ and λ_S, respectively; or $\lambda=\langle V|\mathcal{M}|V\rangle$ and $\lambda_S=\langle V_S|\mathcal{M}_S|V_S\rangle$. We will prove that both λ and λ_S must have the same signature.

First of all,

$$\lambda_S=\mathrm{Min}_v\left[\frac{\langle v|\mathcal{M}_S|v\rangle}{\langle v|v\rangle}\right]=\mathrm{Min}_v\left[\frac{\langle v|\mathcal{M}|v\rangle}{\langle v|S^2|v\rangle}\right]\ .$$

Thus, if λ_S is negative, then negative values for $\langle v|\mathcal{M}|v\rangle$ must exist; therefore λ must be negative. Conversely, from

$$\lambda = \mathrm{Min}_v \left[\frac{\langle v|\mathcal{M}|v\rangle}{\langle v|v\rangle} \right] = \mathrm{Min}_v \left[\frac{\langle v|\mathcal{M}_S|v\rangle}{\langle v|S^{-2}|v\rangle} \right],$$

one similarly concludes that if λ is negative, then λ_S must be negative.

If either λ or λ_S is zero, so too must the other. Assume that λ is zero, then from the above analysis it follows that λ_S must be zero or negative. However, if the latter is true, then λ must be negative, which results in a contradiction. Clearly then, if either λ or λ_S is positive, so too must the other. Thus we see that both λ and λ_S must have identical signatures.

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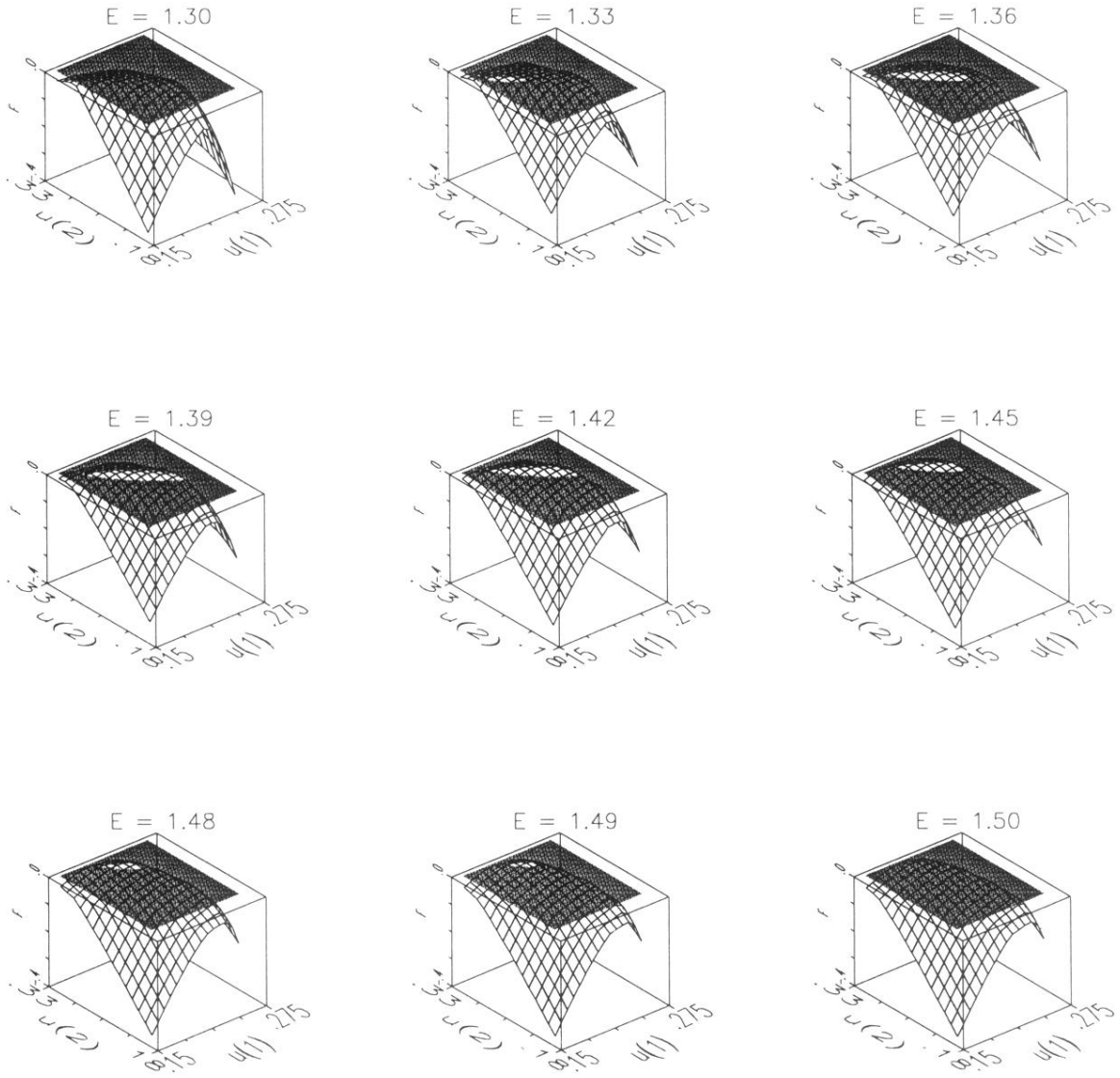

FIG. 1. Side view of the emergence and submergence of the volcano function for the sextic oscillator potential problem ($m=g=1$). The maximum moment order $P_{\max}$ is 6.