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Approximate shape-invariant potentials in quantum mechanics

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Abstract. We introduce and explore the concept of approximate shape invariance of parametrized potential functions for non-relativistic one-dimensional quantum systems. The supersymmetric partner V_2 of an approximate shape-invariant potential V_1 does not exhibit the same shape as the original potential. However, by an appropriate choice of the values of the relevant parameters, V_2 can still be approximated by V_1. We also propose a measure for the degree of shape invariance exhibited by a parametrized potential function. In order to illustrate these ideas we consider (a) the Lillo–Mantegna potentials admitting exact analytic power-law ground-state wavefunctions, and (b) a family of potentials whose ground-state eigenfunctions are given by the trial wavefunctions employed by Cooper, Dawson and Shepard in the SUSY-based variational method.

1. Introduction

The applications of supersymmetry ideas to non-relativistic quantum mechanics developed during the last 15 years have shed new light on many aspects of this branch of physics [1]. The supersymmetry approach to quantum mechanics has provided a deeper understanding of the analytically solvable Hamiltonians as well as a powerful set of new approximation schemes for dealing with problems admitting no exact solution [1–14]. The supersymmetry techniques have found interesting applications in atomic [15–17], nuclear [18–20] and condensed matter physics [21].

The concept of shape invariance plays a fundamental role in the application of supersymmetry methods to quantum mechanics [2–14]. It constitutes the basis of both (a) a unified treatment of all the already known textbook cases of potentials admitting analytical solution and (b) a systematic procedure to generate new exactly solvable systems.

The aims of this paper are:

(a) to consider the application of the supersymmetric approach to quantum systems that are not shape invariant but, in spite of this, are still endowed with this symmetry, albeit in an approximate fashion; and
(b) to introduce a measure of the degree of shape invariance exhibited by a given parametrized family of potentials.

The paper is organized as follows. In section 2 we provide a brief review of the basic notions of the quantum mechanical supersymmetric formalism. In section 3 we consider the

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concept of approximate shape-invariant (ASI) potentials and illustrate it by recourse to the Lillo–Mantegna family of potentials exhibiting exact, power-law ground-state wavefunctions [22]. In section 4 we introduce a measure for the degree of shape invariance. This measure is computed numerically both for the Lillo–Mantegna potentials and for the potentials associated with the Cooper–Dawson–Shepard trial wavefunctions. Finally, some conclusions are drawn in section 5.

2. Quantum mechanics, supersymmetry and shape invariance

In this section we give a brief review of the supersymmetry and shape-invariance ideas as applied to the one-dimensional Schrödinger equation (see [1] for a comprehensive review on this subject). The quantum mechanical supersymmetric formalism revolves around specific relations between the eigenenergies, eigenfunctions and phase shifts of the two Hamiltonians

$$H_{1,2} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_{1,2} \tag{1}$$

associated with the two supersymmetric partner potentials V_1 and V_2. The ground-state energy of H_1 is assumed to be zero. The Hamiltonian operators $H_{1,2}$ are factorized as

$$\begin{aligned} H_1 &= A^\dagger A \\ H_2 &= A A^\dagger. \end{aligned} \tag{2}$$

The operators

$$\begin{aligned} A &= \frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}}{\mathrm{d}x} + W \\ A^\dagger &= -\frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}}{\mathrm{d}x} + W \end{aligned} \tag{3}$$

are given in terms of the so-called quantum superpotential $W(x)$, which is related to the potential functions $V_{1,2}$ by

$$V_1 = W^2 - \frac{\hbar W'}{\sqrt{2m}} \qquad V_2 = W^2 + \frac{\hbar W'}{\sqrt{2m}} \tag{4}$$

the prime denoting derivative with respect to x.

The partner Hamiltonians H_1 and H_2 have exactly the same energy spectra, except for the fact that H_2 has one bound state less than H_1 [1]. The eigenenergies and eigenstates of the partner Hamiltonians $H_{1,2}$ are related by

$$\begin{aligned} E_0^{(1)} &= 0 \\ E_n^{(2)} &= E_{n+1}^{(1)} \qquad (n = 0, 1, \ldots) \end{aligned} \tag{5}$$

and

$$\begin{aligned} \left(E_{n+1}^{(1)}\right)^{-1/2} A \psi_{n+1}^{(1)} &= \psi_n^{(2)} \\ \left(E_n^{(2)}\right)^{-1/2} A^\dagger \psi_n^{(2)} &= \psi_{n+1}^{(1)} \qquad (n = 0, 1, \ldots). \end{aligned} \tag{6}$$

The superpotential W can be obtained from the ground-state wavefunction of H_1 as

$$W(x) = -\frac{\hbar}{\sqrt{2m}}\frac{1}{\psi_0^{(1)}}\frac{\mathrm{d}\psi_0^{(1)}}{\mathrm{d}x}. \tag{7}$$

The concept of shape invariance constitutes the basis of a powerful and elegant generalization of the well known procedure for solving the harmonic oscillator using raising and lowering operators. A potential $V(x; a)$ depending on a set of parameters a is said to be shape invariant when it is related to its supersymmetric partner by the integrability condition [1, 6, 7]

$$V_2(x; a_1) = V_1(x; a_2) + R(a_1). \tag{8}$$

The parameters a_2 are function of the parameters a_1,

$$a_2 = f(a_1) \tag{9}$$

and $R(a_1)$ is an x-independent potential shift. The energy eigenvalues and eigenfunctions of shape-invariant potentials can be obtained in an algebraic fashion. In order to do this one has to consider the hierarchy of Hamiltonians H_i $(i = 1, 2, \ldots)$, where H_{i+1} is the supersymmetric partner of H_i. The potential functions of successive supersymmetric partners of the hierarchy are related by

$$V_{i+1}(x; a_i) = V_i(x; a_{i+1}) + R(a_i). \tag{10}$$

The eigenenergies of a shape-invariant potential are then given in the fashion [1]

$$E_n = \sum_{i=1}^{n} R(a_i) \tag{11}$$

where

$$a_{i+1} = f(a_i) \qquad (i = 1, \ldots, n-1). \tag{12}$$

All the usual exactly solvable potentials, as well as many other recently discovered ones, belong to the class of shape-invariant potentials [1].

3. Approximate shape-invariant potentials

We will say that the family of potential functions $V_1(x; a)$ parametrized by the set of parameters a is *approximately* shape invariant if there exists an appropriate function $a_2 = f(a_1)$ such that

$$V_2(x; a_1) \simeq V_1(x; a_2) + R(a_1). \tag{13}$$

A simple but instructive illustration of the concept of approximate shape invariance that we introduce here is provided by the family of one-dimensional potentials endowed with the exact (normalized) power-law ground-state wavefunctions

$$\psi_0(x; q, \beta) = K(q, \beta)^{1/2} [1 - (1-q)\beta x^2]^{\frac{1}{2(1-q)}} \tag{14}$$

where the normalization factor $K^{1/2}$ is given by

$$K(q, \beta) = \frac{1}{2}(3-q)\frac{\Gamma\left[\frac{1}{2} + [1/(1-q)]\right]}{\Gamma[1/(1-q)]}\sqrt{\frac{(1-q)\beta}{\pi}} \tag{15}$$

and q and β are appropriate parameters. We are going to consider only values of the parameters q and β such that $(1-q)\beta > 0$. In that case, the wavefunction (14) is defined within the interval of x-values corresponding to non-negative values of the quantity between brackets in (14) (for more details see the comments after equation (16)). The probability density $\rho = |\psi_0|^2$ associated with the above wavefunctions has a Tsallis maximum entropy form [23]. These

kinds of distributions provide useful generalizations of the Gaussian distribution that have already found interesting applications in a variety of fields (see [24] and references therein).

It is easy to verify that the potential admitting (14) as ground-state wavefunction is given by (from now on we take $\hbar = 1$ and $m = 1$)

$$V_1 = \frac{1}{2}\frac{q\beta^2x^2 - \beta}{[1-(1-q)\beta x^2]^2} = W^2 - \frac{1}{\sqrt{2}}W'. \tag{16}$$

We will restrict our considerations to values of the Tsallis parameter q belonging to the interval $(\frac{1}{2}, 1)$, and to positive values of β. For these values of the parameters the potential V_1 exhibits two singularities (that is, infinite walls) at

$$x_{1,2} = \pm\sqrt{\frac{1}{(1-q)\beta}} \tag{17}$$

and has, consequently, an infinite number of bound states. The concomitant wavefunctions are defined within the interval $[x_1, x_2]$ and vanish at its extreme points. In particular, the ground-state wavefunction (14) clearly vanishes at $x_{1,2}$. In the limit case $q \to 1$ the two points $x_{1,2}$ corresponding to the singularities of the potential V_1 go to $\pm\infty$ and a harmonic oscillator potential with natural angular frequency β is obtained. Quantum potentials exhibiting (after an appropriate identification of parameters) the form (16), corresponding to $q > 1$, were recently introduced by Lillo and Mantegna [22] in connection with the dynamical evolution of non-Gaussian wavepackets.

The quantum superpotential W associated with V_1 can be determined from the ground-state wavefunction by recourse of equation (7), yielding

$$W = \frac{\beta}{\sqrt{2}}\frac{x}{[1-(1-q)\beta x^2]} \tag{18}$$

which, applying equation (4), allows us to determine the supersymmetric partner potential

$$V_2 = \frac{1}{2}\frac{(2-q)\beta^2x^2 + \beta}{[1-(1-q)\beta x^2]^2} = W^2 + \frac{1}{\sqrt{2}}W'. \tag{19}$$

If V_1 were shape invariant there would exist appropriate functions

$$q' = q'(q, \beta) \tag{20}$$

and

$$\beta' = \beta'(q, \beta) \tag{21}$$

such that

$$V_2(q, \beta) = V_1(q', \beta') + R(q, \beta) \tag{22}$$

with R independent of x. Unfortunately, that is not the case. However, it is still possible to find a parameter transformation (20) and (21) yielding an *approximate* shape-invariant relation defined by

$$V_2(q, \beta) \simeq V_1(q', \beta') + R(q, \beta) \tag{23}$$

with R independent of x; that is,

$$V_2 = \frac{1}{2}\frac{(2-q)\beta^2x^2 + \beta}{[1-(1-q)\beta x^2]^2} \simeq \frac{1}{2}\frac{q'\beta'^2x^2 - \beta'}{[1-(1-q')\beta' x^2]^2} + R. \tag{24}$$

As we shall see in section 4, an optimum transformation (20) and (21) can be determined numerically by recourse to the maximization of the overlap between the ground-state wavefunctions associated with the potentials $V_2(q, \beta)$ and $V_1(q', \beta')$. It will prove instructive, however, to consider first a simple analytical version of the transformation (20) and (21) that, although it is not the optimal one, (a) yields a very good approximation for the energy of the first excited state of $V_1(q, \beta)$, (b) illustrates some important aspects of the approximate shape-invariant character of this potential, and (c) provides a useful starting point for the analysis of the optimal transformation.

In order to determine a simple (albeit not necessarily optimal) analytical ASI transformation (20) and (21) it is reasonable to require that both $V_2(q, \beta)$, and its approximation $V_1(q', \beta') + R(q, \beta)$, should have their respective singularities located at the same positions. Consequently, we obtain the relation

$$(1 - q')\beta' = (1 - q)\beta. \tag{25}$$

If we also demand that both V_2 and its approximation behave in the same way at their singularities (that is, we require that the numerators of both $V_2(q, \beta)$ and $V_1(q', \beta')$ attain the same value at the singularities) we obtain a second relation, namely,

$$\frac{(2 - q)\beta}{(1 - q)} + \beta = \frac{q'\beta'}{(1 - q')} - \beta'. \tag{26}$$

These requirements lead to a quadratic equation for q'

$$[3 - 2q](1 - q')^2 + 2(1 - q)^2(1 - q') - (1 - q)^2 = 0 \tag{27}$$

whose solutions are given by

$$(1 - q') = [(q - 1) \pm (q - 2)]\frac{(1 - q)}{3 - 2q}. \tag{28}$$

Since, on one hand, $\frac{1}{2} < q < 1$, and, on the other, we wish for $1 - q' > 0$, we choose the minus sign and arrive at

$$q' = \frac{2 - q}{3 - 2q}. \tag{29}$$

Note that

$$\begin{aligned} &q = 1 \to q' = 1 \\ &q = \tfrac{1}{2} \to q' = \tfrac{3}{4} \\ &q \in \left(\tfrac{1}{2}, 1\right) \to q' \in \left(\tfrac{3}{4}, 1\right). \end{aligned} \tag{30}$$

We determine β' according to

$$\beta'(1 - q') = \beta(1 - q) \tag{31}$$

which leads to

$$\beta' = (3 - 2q)\beta. \tag{32}$$

The analytical approximate shape-invariance scheme described by the transformations (29) and (32) was obtained by requiring that both $V_2(q, \beta)$ and $V_1(q', \beta')$ exhibit the same asymptotic behaviour at their (common) singularities $x_{1,2}$ (see equation (17)). From now on we shall

call this simple ASI scheme the asymptotic shape-invariant scheme (asymptotic ASI scheme). Now, using (16), (19), (29) and (32) we write

$$V_1(q', \beta')|_{x=0} = \frac{1}{2}(2q - 3)\beta \tag{33}$$

and

$$V_2(q, \beta)|_{x=0} = \frac{\beta}{2} \tag{34}$$

so that, in order that $V_1(q', \beta')$ and $V_2(q, \beta)$ coincide at the bottom of the potential well, we need to add to $V_1(q', \beta')$ the quantity

$$R = \beta(2 - q) \tag{35}$$

i.e.

$$V_2(q, \beta) \simeq V_1(q', \beta') + \beta(2 - q). \tag{36}$$

When $q = 1$ we find that (a) $q' = q$, (b) $\beta' = \beta$ and (c) equation (36) reduces to the exact shape-invariance relation of the harmonic oscillator. Let us consider what happens in the general case $q \in (\frac{1}{2}, 1)$. Since (a) $E_0^{(2)} = E_1^{(1)}$ and (b) the ground state of $V_1(q, \beta)$ (or of $V_1(q', \beta')$) vanishes, we find that the first excited energy level of V_1 is

$$E_1^{(1)} = E_0^{(2)} \simeq \beta(2 - q). \tag{37}$$

The second energy level will be given by

$$E_2^{(1)} \simeq \beta(2 - q) + \beta'(2 - q'). \tag{38}$$

Let us now find the general expression for the eigenvalues $E_1^{(n)}$ within the present asymptotic ASI scheme. We have

$$E_n^{(1)} \simeq \sum_{i=0}^{n-1} R(\beta^{(i)}, q^{(i)}) \tag{39}$$

$$= \sum_{i=0}^{n-1} \beta^{(i)}(2 - q^{(i)}) \tag{40}$$

where $\beta^{(0)}$ and $q^{(0)}$ denote the starting set of parameters (that is, those characterizing V_1), $\beta^{(1)} = \beta'$, $q^{(1)} = q'$, and

$$\begin{aligned} q^{(i+1)} &= \frac{2 - q^{(i)}}{3 - 2q^{(i)}} \\ \beta^{(i+1)} &= (3 - 2q^{(i)})\beta^{(i)}. \end{aligned} \tag{41}$$

Now, because of equation (31), we have $\beta(1 - q) = C = \text{constant}$. Hence we can write

$$R = C\, p \qquad \text{where} \quad p = (2 - q)/(1 - q). \tag{42}$$

Equations (29) and (32), that define the transformation laws for β and q, imply that the parameter p obeys the simple transformation rule

$$p' = p + 2. \tag{43}$$

Consequently, the energy levels provided by the asymptotic ASI scheme are

$$E_n^{(1)} \simeq C\left[np + \sum_{i=1}^{n-1} 2i\right]$$
$$= Cn(p-1) + Cn^2. \tag{44}$$

In the above equation $p = (2-q)/(1-q)$ denotes the starting value of this parameter. It can be verified from equations (42) and (43) that the result of performing n times the (q, β) transformation defined by equations (29) and (32) is given by

$$q^{(n)} = 1 - \frac{1-q}{1+2n(1-q)} \tag{45}$$

and

$$\beta^{(n)} = \beta[1+2n(1-q)]. \tag{46}$$

It follows from (45) that $\lim_{n\to\infty} q = 1$. This means that the hierarchy of approximate shape-invariant potentials obtained by the successive application of the (q, β)-map (29)–(32) relaxes, for large values of n, to a harmonic oscillator potential. However, since $\lim_{n\to\infty} \beta = \infty$, the frequency of the limiting harmonic oscillator diverges. The combined behaviours of q and β lead, for large n, to an infinite square-well-like spectra with energy levels growing as n^2 (see equation (44)).

An improved implementation of the asymptotic ASI scheme, leading to a better approximation for the energy eigenvalues, can be obtained by recourse to a first-order perturbation correction. In our example, the supersymmetric partner potential $V_2(q, \beta)$ is approximated by a potential $V_1(q', \beta')$ with the same shape as the original one but with appropriately chosen new parameters. The essential point is that we know exactly the ground-state energy and wavefunction of $V_1(q', \beta')$. In order to determine a better approximate value for the ground-state energy of $V_2(q, \beta)$ we can consider $V_1(q', \beta')$ as our 'unperturbed' potential, and regard the difference

$$\Delta V(x) = V_2(x; q, \beta) - V_1(x; q', \beta') \tag{47}$$

as a small perturbation. The concomitant first-order correction to the ground-state energy of V_2 which, in turn, also constitutes a correction to the first excited energy level of V_1, is

$$\Delta E_1^{(1)} = \langle \psi_0(x; q', \beta') | \Delta V | \psi_0(x; q', \beta') \rangle$$
$$= \beta(2-q)\, K(q', \beta') \left[\int [1-(1-q)\beta x^2]^{\frac{q'}{1-q'}}\, \mathrm{d}x\right] - \beta(2-q). \tag{48}$$

The above expression leads, after some algebra, to an improved value for $E_1^{(1)}$ given by

$$\tilde{E}_1^{(1)} = \beta(2-q) + \Delta E$$
$$= \frac{1}{2}\beta(2-q)\left[\frac{7-5q}{3-2q}\right]. \tag{49}$$

This new (and better) approximation for $E_1^{(1)}$ allows us to formulate an improved version of our asymptotic ASI scheme, based on a new choice for the quantity $R(q, \beta)$ appearing in the approximate shape-invariance relation (23). We now adopt

$$\tilde{R}(q, \beta) = \frac{1}{2}\beta(2-q)\left[\frac{7-5q}{3-2q}\right]. \tag{50}$$

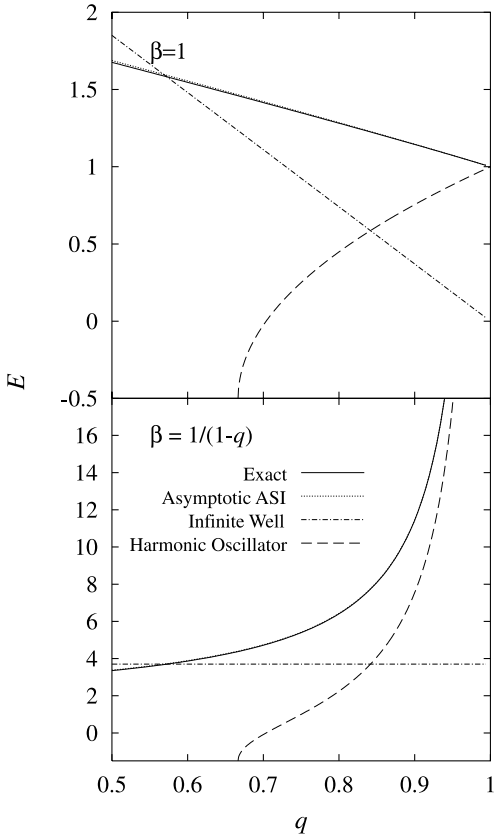

Figure 1. Plots of the exact first excited eigenenergy of $V_1(q, \beta)$ and the first excited state eigenenergies corresponding to: (a) the asymptotic ASI scheme, (b) a harmonic oscillator fitting the bottom of the potential and (c) an infinite square well with its walls located at the singular points of $V_1(q, \beta)$.

The approximate energy eigenvalues provided by the new asymptotic ASI scheme are

$$\tilde{E}_n^{(1)} = \sum_{i=0}^{n-1} \tilde{R}(q^{(i)}, \beta^{(i)}). \tag{51}$$

The exact eigenenergies of the first excited state of V_1, as well as the approximated ones yielded by the improved asymptotic ASI scheme, are plotted in figure 1 as a function of q. The first excited eigenenergies corresponding to (a) infinite square wells having their 'walls' located at the singular points of V_1, and (b) harmonic oscillator potentials, fitting the potential function V_1 at $x = 0$, are also depicted. In these last two cases the potentials were shifted in order to make their ground-state eigenenergies equal to zero. The first excited state energy eigenvalues provided by the asymptotic ASI scheme are seen to be in very good agreement with the numerically computed exact ones. The success of the simple asymptotic ASI scheme constitutes a clue indicating that the parametrized potential $V(q, \beta)$ is endowed, to a remarkable degree of approximation, with the symmetry of shape invariance. A different kind of ASI scheme can be obtained by comparing the Taylor expansion of both $V_2(q, \beta)$ and $V_1(q', \beta') + R(q, \beta)$ around $x = 0$. The quantities q', β' and R are, in this case, those that make the first three non-vanishing coefficients of the above-mentioned Taylor expansion coincide. This procedure also leads to closed analytical expressions for both q' and β', albeit considerably more complicated than those provided by the asymptotic ASI scheme. In the next section we shall determine, in numerical fashion, the optimum ASI map (20) and (21).

4. The optimal ASI parameter transformation

4.1. A measure of the degree of shape invariance

Let us consider a family of normalized wavefunctions

$$\Psi_0^{(1)}(x;\alpha) \tag{52}$$

parametrized by the set of parameters α. The $\Psi_0^{(1)}(x;\alpha)$s are regarded as the ground-state wavefunctions of a corresponding family of one-dimensional parametrized potentials $V_1(x;\alpha)$. Using the functions (52) it is possible to obtain the associated superpotentials $W(x;\alpha)$ and the concomitant supersymmetric partner potentials $V_2(x;\alpha)$. Now, let $\Psi_0^{(2)}(x;\alpha)$ be the (exact) ground-state wavefunctions of the partner potentials. A simple but important consequence of the shape-invariance integrability condition (8) is that it can be reformulated in terms of the ground-state wavefunctions associated with the potentials $V_{1,2}$. The two potentials appearing in the shape-invariance relation (8) have the same form, differing only in the constant energy shift R. Hence, the shape-invariance condition (8) implies the existence of an appropriate set of parameters α' such that the ground-state wavefunctions associated, respectively, with $V_2(x;\alpha)$ and $V_1(x;\alpha')$, are the same. More explicitly,

$$\Psi_0^{(2)}(x;\alpha) = \Psi_0^{(1)}(x;\alpha'). \tag{53}$$

On the basis of the above considerations we here propose to use, as a measure of the degree of shape invariance of the family of potentials $V_1(x;\alpha)$, the quantity

$$\begin{aligned} I(\alpha) &= \max_{\{\alpha'\}} \langle \Psi_0^{(1)}(\alpha') \mid \Psi_0^{(2)}(\alpha) \rangle \\ &= \max_{\{\alpha'\}} \int \Psi_0^{(1)}(x;\alpha')\, \Psi_0^{(2)}(x;\alpha)\, \mathrm{d}x. \end{aligned} \tag{54}$$

The meaning of $I(\alpha)$ is clear. It measures how well the ground state of the supersymmetric partner potential $V_2(x;\alpha)$ can be represented by an appropriately chosen member of the original family of wavefunctions (52). Note that the above measure of shape invariance depends itself on α. By definition, the parametrized potential $V_1(x;\alpha)$ is shape invariant if

$$I(\alpha) = 1 \tag{55}$$

for all values of the parameter α. If this is not the case, the set of parameters α' provided by (54) determine the optimal ASI scheme associated with the family of potentials $V_1(x;\alpha)$ (or, equivalently, the best ASI scheme associated with the wavefunctions $\Psi_0^{(1)}(x;\alpha)$). In the next two subsections we are going to apply these ideas to two particular examples: (a) the family of Tsallis MaxEnt wavefunctions and (b) the variational ansatz of Cooper, Dawson and Shepard (CDS) [8].

4.2. Tsallis MaxEnt wavefunctions

We have computed numerically, for the parametrized family of Tsallis MaxEnt wavefunctions (14), the values of the parameters $q'(q,\beta)$ and $\beta'(q,\beta)$ that maximize the overlap (54). These two functions provide, for the family of potentials (16), the optimal ASI map (20) and (21). In order to verify how well the potentials $V_1(q,\beta)$ comply with the shape-invariance symmetry, we can compare the (approximate) eigenenergies obtained from the optimal ASI scheme with the numerically computed exact ones. Two ingredients are needed for the approximate evaluation of the energy eigenvalues on the basis of the ASI scheme (see equation (39)). On one hand, the optimal ASI map (obtained by the overlap maximization procedure) is required. On the

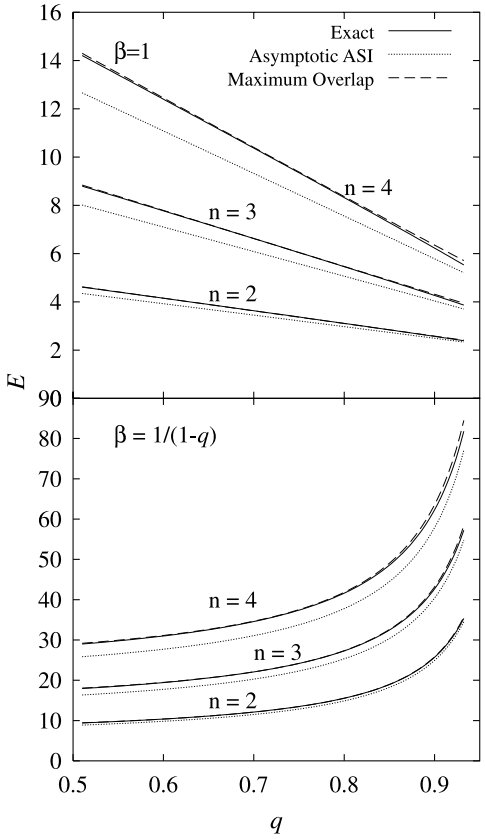

Figure 2. Plots of the exact $E_2^{(1)}$, $E_3^{(1)}$ and $E_4^{(1)}$ eigenenergies of $V_1(q, \beta)$ and of the corresponding approximations obtained by recourse of (a) the asymptotic ASI scheme and (b) the optimal ASI transformations.

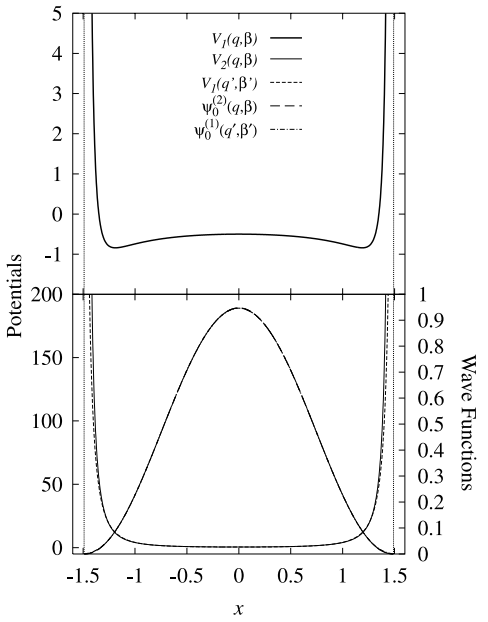

Figure 3. The potential V_1 corresponding to a value $q = 0.55$ of the Tsallis parameter and to $\beta = 1$ (upper figure) and the associated partner potential V_2, its optimal ASI approximation, and their respective ground-state eigenfunctions (lower figure).

other hand, we need an appropriate expression for $R(q, \beta)$. Remember that $R(q, \beta)$ is just the energy $E_1^{(1)}$ of the first excited state of $V_1(q, \beta)$. As we have seen in section 3, the asymptotic ASI scheme yields a very good approximation for $E_1^{(1)}$, namely, equation (50). Consequently, the energy eigenvalues $E_n^{(1)}$ of $V_1(q, \beta)$ can be computed by inserting into (51) the optimal ASI transformation and then adopting, for $R(q, \beta)$, the expression (50) for the first excited eigenenergy $E_1^{(1)}$ provided by the asymptotic ASI scheme.

The exact eigenenergies $E_2^{(1)}$, $E_3^{(1)}$ and $E_4^{(1)}$ obtained by numerically solving the Schrödinger equation are compared in figure 2 with (a) the eigenenergies yielded by the asymptotic ASI scheme and (b) the eigenenergies associated with the optimal ASI map. As was already explained, the energy values provided by the optimal ASI map were computed as if the potential $V_1(q, \beta)$ were shape invariant. The agreement between these ASI eigenenergies and the exact ones is, again, very good. This means that, even if the parametrized family of potentials $V_1(q, \beta)$ is not shape invariant, it is nevertheless endowed with this symmetry to a high degree of approximation. In the upper panel of figure 3 we exhibit the shape of $V_1(q, \beta)$ for $q = 0.55$ and $\beta = 1$. In the lower panel of that figure we compare the potential $V_2(q, \beta)$ with its optimal ASI approximation $V_1(q', \beta') + R(q, \beta)$. The ground-state wavefunctions

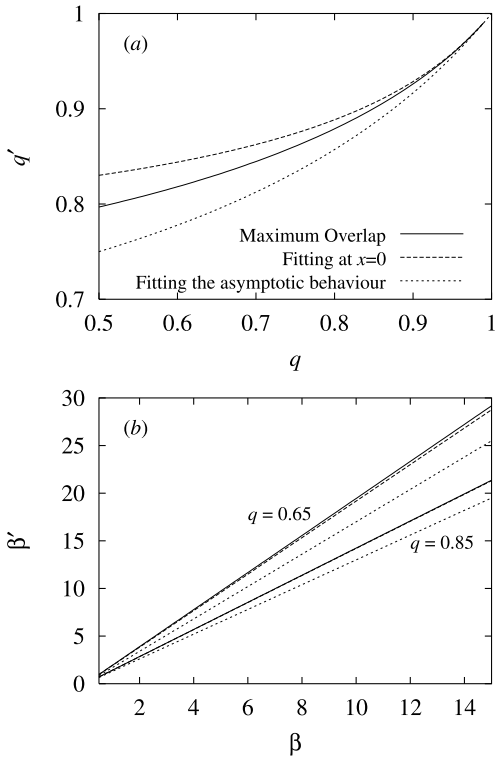

Figure 4. The ASI maps obtained from (a) the asymptotic ASI scheme, (b) the fitting of the first three terms of the Taylor series expansion around $x = 0$ of V_2 and of its ASI approximation and (c) by the maximization of the overlap $I(q, \beta)$ (see equation (54)).

associated with these two potentials are also depicted. The potential V_2 closely resembles its ASI approximation for almost the entire range of allowed x-values. The potential V_2 starts to differ from its approximation only when we approach the singularities of V_2. The ground-state wavefunctions of V_2 and of its ASI approximation are also seen to be of quite similar character.

The ASI maps $q'(q)$ and $\beta'(q, \beta)$ are depicted, respectively, in figures 4(*a*) and (*b*). Those figures depict the ASI maps calculated by recourse to:

(a) maximizing the overlap between the ground-state wavefunctions of V_2 and its ASI approximation;
(b) the asymptotic ASI scheme; and
(c) fitting the first three terms of the Taylor expansion around $x = 0$ of both V_2 and its ASI approximation.

Our calculations indicate that $q'(q)$ does not depend on β.

4.3. The Cooper–Dawson–Shepard wavefunctions

As a second example of our concept of approximate shape invariance we are now going to compute the shape-invariant measure I corresponding to the family of ground-state wavefunctions

$$\Phi_0 = N \exp\left(-b|x|^{2a}\right) = N \exp\left(-b(x^2)^a\right) \tag{56}$$

which are parametrized by the two real numbers a and b ($N = N(a, b)$ is a normalization factor). (An interesting study of shape-invariant potentials that depend upon n parameters is that of Cariñena and Ramos [25].) The wavefunctions (56) have been recently applied as a trial variational ansatz within the SUSY-based variational method recently proposed by CDS [8]. Before analysing the degree of shape invariance of the family (56) it is worth briefly reviewing the CDS approach, since interesting connections can be established between the concept of an approximate shape invariant, on one hand, and the SUSY-based variational method, on the other. The essence of the CDS scheme boils down to the following procedure. Given an appropriate variational ansatz, the approximate ground-state eigenenergies and eigenfunctions of a potential V_1 are computed in the usual way. The approximate ground-state wavefunction is then used to determine the superpotential W and, from W, the supersymmetric partner V_2. Then, the variational ansatz is used again, this time to determine an approximate ground-state wavefunction for V_2. Finally, an approximated first excited state for V_1 is obtained by recourse to equation (6). A similar procedure can be applied once again in order to determine higher-order excited states. The CDS method differs from the standard one in the way in which the variational approximation for the excited states is dealt with. Within the CDS approach, one does not perform a constrained variational procedure in order to guarantee the orthogonality of the eigenstates. Instead, one always deals with the unconstrained variational computation of the ground states associated with a supersymmetric hierarchy of potentials [8]. In [8] the CDS method was applied to the anharmonic oscillator using for the ground-state wavefunction the ansatz (56). It was shown in the above referred to paper that the CDS scheme provides good approximations for low-n excited states, but the approximation deteriorates when higher excited states are considered.

The superpotential associated with the parametrized ground-state wavefunction (56) is

$$W = \sqrt{2}\, ab\, x\, (x^2)^{a-1}. \tag{57}$$

The concomitant partner potentials are thus given by

$$V_1 = 2a^2b^2(x^2)^{2a-1} - (2a-1)ab(x^2)^{a-1} \tag{58}$$

and

$$V_2 = 2a^2b^2(x^2)^{2a-1} + (2a-1)ab(x^2)^{a-1}. \tag{59}$$

Since V_1 is not a shape-invariant potential, the ground-state wavefunction $\Psi_0^{(2)}$ of V_2 cannot be exactly described by the ansatz (56). In order to evaluate the shape-invariance measure $I(a, b)$ (see (54)), we have to find special values (a', b') of the parameters a, b that yield the wavefunction of the form (56) that provides the best representation of $\Psi_0^{(2)}$. This is achieved by maximizing the overlap of such a wavefunction with $\Psi_0^{(2)}$ (the exact ground-state wavefunction $\Psi_0^{(2)}$ of V_2 was obtained numerically by solving the concomitant Schrödinger equation by recourse to a standard numerical algorithm). The results of this extremizing process are illustrated in figures 5 and 6. The optimum parameters (a', b') are depicted in figure 5 as a function of the original parameters (a, b). It was found numerically that neither the parameter a' nor the measure I depend on b. On the other hand, b' depends on both a and b. The optimum overlap $I(a)$ is plotted in figure 6. The overlap $I(a)$ (for $a > 1$) is a monotonically decreasing function of a, but remains, always, quite close to unity. This constitutes part of the explanation of the success exhibited by the wavefunctions (56) as a trial variational ansatz within the CDS SUSY-based variational method.

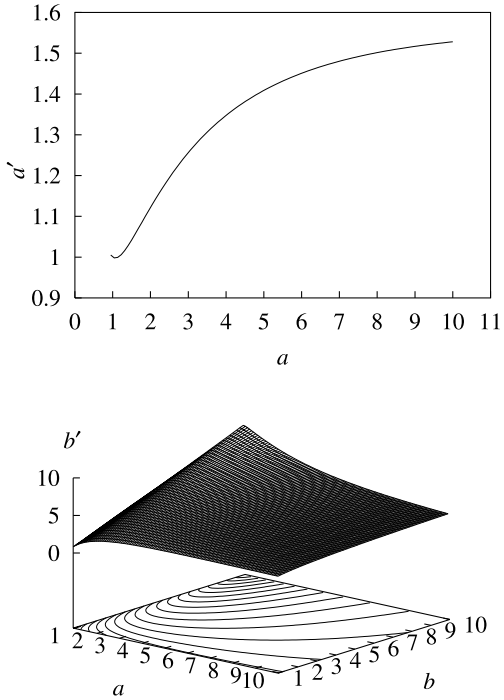

Figure 5. The optimal ASI maps $a'(a)$ and $b'(a, b)$ for the family of wavefunctions (56), obtained by recourse to the maximization of the overlap $I(a, b)$ (see text).

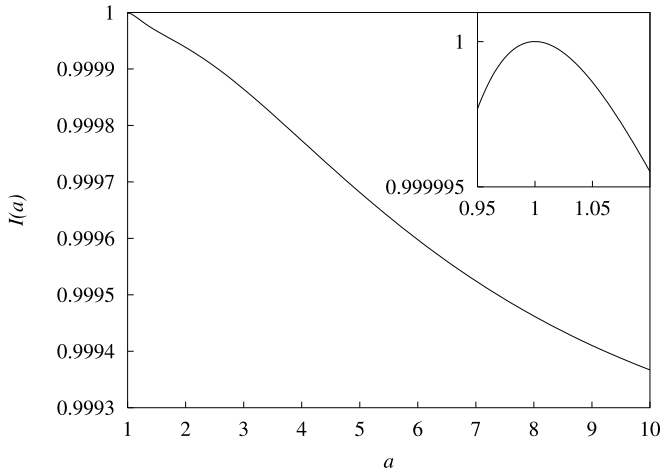

Figure 6. The maximum value of the overlap $I(a)$ (see equation (54)) associated with the CDS parametrized family of wavefunctions (56).

4.4. Some general comments on approximate shape-invariant potentials

The two examples of approximate shape invariance discussed in this paper illustrate various aspects of this concept. In the case of the Lillo–Mantegna potentials (and their associated Tsallis ground-state wavefunctions) we were able to obtain, from the analytical form of the partner potentials V_1 and V_2, a simple explicit expression for an ASI parameter transformation (20) and (21). However, we may have a parametric family of potentials exhibiting a high

degree of shape invariance even if we do not know an explicit expression for the concomitant ASI transformation. The measure of shape invariance I that we have advanced in this paper provides a useful tool for numerically assessing the degree of shape invariance of a given family of potentials (or a given family of ground-state wavefunctions). As an illustration of this procedure we have computed numerically the measure I associated with the CDS wavefunctions (57), finding that these wavefunctions (or the associated potentials (58)) are indeed endowed with an approximate shape invariance. We also obtained, in numerical fashion, the best ASI parameter transformation, which is exhibited in figure 5. This kind of graph provides useful information concerning the relationship between the eigenfunctions corresponding, respectively, to the original potentials and to their supersymmetric partners. In the case of the CDS example, it is clear from figure 5 that the best ASI transformation associated with the CDS wavefunctions may be approximated by simple analytical expressions (such as those discussed in connection with the Lillo–Mantegna potentials).

We believe that our measure of shape invariance I may constitute the basis of a set of numerical tools which are adequate for studying the shape-invariance properties of families of potentials (as we exemplified with the CDS ansatz). In those cases where there is numerical evidence for a high degree of (approximate) shape invariance, the numerical results obtained (for instance, the optimal ASI transformation) may provide useful clues for the obtention of explicit analytical ASI transformations (such as (20) and (21)). A suggestive analogy with the study of integrable classical Hamiltonian systems can be established here. It is well known that the numerical integration of the concomitant classical equations of motion may provide one with important evidence concerning the integrability of certain systems. There are various numerical tools, like the computation of Poincaré surfaces of section, or the computation of Lyapunov exponents, that can be used for this task. As a matter of fact, there have been important instances of classical Hamiltonian systems whose integrability was first suspected on the basis of numerical evidence. The celebrated Toda lattice constitutes a famous example [26].

One would like to have simple criteria to know in advance whether (or, at least, some hints to formulate educated guesses as to whether) a given parametric family of potentials is endowed with the property of approximate shape invariance. This problem has some similarities with the problem of finding a good ansatz for trial wavefunctions in connection with variational approximate methods. Indeed, as was already mentioned, the search for approximate shape-invariant families of potentials (or ground-state wavefunctions) is closely related to the problem of implementing the SUSY-based variational method. A systematic study of particular families of potentials, with the aid of the numerical procedures that we have already applied when we considered the CDS ansatz, seems to be an indispensable first step in order to obtain further insights in connection with the general characterization of approximate shape-invariant potentials. An interesting possibility for further research is provided by the family of ground-state wavefunctions depending on the three parameters a, b and q, given by

$$\phi_0(x) = D(a,b,q)\left[1-(1-q)\beta\left(x^2\right)^a\right]^{1/2(1-q)} \tag{60}$$

where $D(a,b,q)$ is an appropriate normalization factor. The CDS ansatz (56) is recovered as a particular case of the above family of parametric wavefunctions in the limit $q \to 1$. Besides, the ground-state wavefunctions of the Lillo–Mantegna potentials correspond to the case $a = 1$. A systematic study of the (approximate) shape-invariance properties of this multiparametric family of potentials will be addressed elsewhere.

5. Conclusions

We have here introduced and investigated the concept of approximate shape invariance for parametrized families of one-dimensional potential functions (or parametrized ground-state wavefunctions) in non-relativistic quantum mechanics. As an illustration, we have studied in some detail the (approximate) shape-invariant features of a family of potentials whose ground-state wavefunctions exhibit a Tsallis MaxEnt form. This family of potentials exhibits a remarkable degree of shape invariance. A simple analytical asymptotic ASI scheme provides very good approximate energies for the first excited states. Higher excited eigenenergies evaluated using the optimum ASI parameter transformation are also in good agreement with the corresponding exact energies obtained by numerically solving Schrödinger's equation. It is worth mentioning that, as far as we know, the Tsallis family of potential functions (16) cannot be obtained by adding a small perturbation δV to a known (exactly) shape-invariant potential. In particular, the potentials (16) cannot be regarded as small perturbations of harmonic oscillator potentials (see figures 1 and 3). As a second example we computed numerically the optimum ASI transformation associated with the parametrized family of wavefunctions used by Cooper *et al* as a trial ansatz within the SUSY-based variational method. This family also exhibits a high degree of shape invariance. These results are fully consistent with the successful performance of the CDS trial wavefunctions within the SUSY-based variational method, as reported in [8].

We believe that further research on the concept of approximate shape invariance may contribute to our understanding of both the exactly solvable and the non-soluble one-dimensional quantum potentials. In particular, it may shed new light on the properties of supersymmetry-inspired approximate methods applied for solving the Schrödinger equation (such as the SUSY-based variational technique).

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