

Construction of stationary quantum states with targeted energies

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Abstract Given an exact stationary state and its energy-eigenvalue, we devise a simple way of generating new families of exact eigenstates with the same eigenenergy, but for different potentials. While this recipe of designing isoergic states is quite general in the context of arriving at new exact solutions from a known premise, relevance of this route with the scheme of construction of isospectral potentials is noted under specific situations. The idea is extended to finding new exact eigenstates with eigenvalues as the sum of energies of two or more separate but known stationary states in dissimilar potentials. Implication of the latter endeavor in the contexts of manifold energy minimization is discussed.

Keywords Stationary states · Isoergic states · Isospectral potentials · Manifold energy

1 Introduction

Given an exact solution of the stationary Schrödinger equation (SE) for a given real potential V_0 and a state n in the form (choosing $\hbar = 1$ and $m = 1/2$)

$$-\Psi''_{n0} + V_0\Psi_{n0} = \varepsilon_{n0}\Psi_{n0}, \quad (1)$$

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we devise a route to obtain another exact solution with the same energy, but for a different real potential V . In other words, we intend to arrive from (1) at

$$-\Phi_m'' + V\Phi_m = E_m\Phi_m, \quad (2)$$

where $E_m = \varepsilon_{n0}$, and states m and n may be same or different. If (2) is already known, the equality $E_m = \varepsilon_{n0}$ may be achieved by supplying a constant shift in V . But, this is a trivial point. Our interest here is to *construct* some nontrivial V and the corresponding Φ_m in (2) from a knowledge of (1) alone such that the energy eigenvalue in (2) remains at ε_{n0} . Secondly, we intend to also explore how, with the help of (1) and (2), one can cook up another energy eigenvalue equation

$$-\Theta'' + V_T\Theta = (E_m + \varepsilon_{n0})\Theta \quad (3)$$

whose energy is seen to be the sum of the energies of the two earlier cases. Thus, attention of the present work is primarily focused on engineering the potential part to get stationary states with pre-assigned energies.

We may note that our first task, in the special situation of $m = n = 0$, has a kinship with the scheme of construction of isospectral potentials in supersymmetric (SUSY) quantum mechanics [1–4]. It has also a bearing on the search for solvable potentials that may give rise to new families of orthogonal polynomials [5]. Our second task of defining a third system with eigenenergy as the sum of two or more given states of different systems is linked to the concept of minimization of manifold energy (MME) [6–8]. Specifically, we may opt for a purely nonlinear variational scheme to minimize the quantity concerned, though the origin of the said notion lies in linear variations. Quasi-ideal mixtures [9, 10] provide another practical case. The idea is easily extendable to more than two states as well. Thus, importance of both the above schemes may be appreciated.

2 The strategy

For convenience, we cast the SE in the form of a nonlinear Riccati equation (RE) [11–16] by defining

$$\chi_{n0} = \Psi'_{n0} / \Psi_{n0}. \quad (4)$$

This transforms (1) to

$$\chi_{n0}^2 + \chi'_{n0} + \varepsilon_{n0} - V_0 = 0. \quad (5)$$

In (1) or (4), we have deliberately put an extra subscript (zero) to indicate that it will serve as the starting point. Similarly, the RE corresponding to (2) is written as

$$\chi_m^2 + \chi'_m + E_m - V = 0, \quad (6)$$

with

$$\chi_m = \Phi'_m / \Phi_m . \tag{7}$$

Let us now demand that a specific χ may be constructed from χ_{n0} by using an auxiliary function $\bar{\chi}$ such that

$$\chi = \chi_{n0} + \bar{\chi} \tag{8}$$

and

$$\chi^2 + \chi' + \varepsilon_{n0} - V = 0. \tag{9}$$

Note that (9) is a special case of (6), but the state is isoergic with the parent one in (5). Now, employing (5) and (8) in (9), we find

$$V = V_0 + 2\chi_{n0}\bar{\chi} + \bar{\chi}' + \bar{\chi}^2. \tag{10}$$

This is one of our key equations. It shows, we can choose our auxiliary function $\bar{\chi}$ to get the required potential that would satisfy (9). We can also get the corresponding eigenstate from (8). Thus, a route to go to (2) from (1) is achieved. The state in (9) is finally fixed by noting the number of nodes obtained from (8).

A more stringent requirement, however, is needed to make V an isospectral partner [17] of V_0 . It says that each of the states of (1) and (2) are isoergic. Thus, on one hand, we would require

$$V = V_0 + 2\chi_{00}\bar{\chi} + \bar{\chi}' + \bar{\chi}^2. \tag{11}$$

to be satisfied [for the ground state of (10)]; on the other hand, for excited states to be isoergic too, we should have identical SUSY partners for the two potentials, i.e.,

$$V_0 - 2\chi'_{00} = V - 2\chi'_0. \tag{12}$$

From (11) and (12), coupled with the relation $\chi_0 = \chi_{00} + \bar{\chi}$, we arrive at

$$\bar{\chi}' = \bar{\chi}^2 + 2\chi_{00}\bar{\chi}. \tag{13}$$

Substituting $\bar{\chi} = -I'/I$, we obtain from (13)

$$I''/I' = 2\chi_{00} = 2\Psi'_{00}/\Psi_{00}. \tag{14}$$

On integration, it leads to

$$I'(x) = \Psi_0^2. \tag{15}$$

This means, unlike (10), one needs to now use a specific $\bar{\chi}$ defined by

$$\bar{\chi}(x) = -\frac{I'(x)}{I(x) + \lambda}, \quad (16)$$

with

$$I(x) = \int_{-\infty}^x \Psi_0^2 dx \quad (17)$$

and a parameter λ that can take any value excluding the range $(-1, 0)$ to avoid any blowing up of the denominator in (16). In this case, finally, we have [17]

$$V = V_0 + 2\bar{\chi}'. \quad (18)$$

The second problem of obtaining a new state with energy as the sum of energies of two given stationary states starts as follows. Suppose now that (5) and (6) are given. We add them up to get

$$\chi_{n0}^2 + \chi_m^2 + \chi'_{n0} + \chi'_m + (\varepsilon_{n0} + E_m) - (V_0 + V) = 0. \quad (19)$$

This can be rearranged to

$$(\chi_{n0} + \chi_m)^2 + (\chi_{n0} + \chi_m)' + (\varepsilon_{n0} + E_m) - (V_0 + V + 2\chi_{n0}\chi_m) = 0. \quad (20)$$

We can next identify (20) as the RE corresponding to (3). The number of nodes in (3) will match the number of isolated singularities in χ_T where

$$\chi_T = \chi_{n0} + \chi_m. \quad (21)$$

Rewriting (20) as

$$\chi_T^2 + \chi'_T + E_T - V_T = 0 \quad (22)$$

the association with (3) follows completely, where $\chi_T = \Theta'/\Theta$. The most interesting part here is concerned with the specific modification of the total potential V_T . This is given by the last term in parentheses in (20). Whereas $\Phi_m\Psi_{n0}$ is an interference term in probability, $\chi_m\chi_{n0}$ is seen to have a similar status in potential. Another significant feature of (22) will become clear from a glance at (21). The latter implies that the total wave function will be a product function. Note that usually we come across wave functions as product functions, and energies as sums, only when the coordinates are unrelated. Here, the situation is altogether different. Yet, a tailor-made potential can be found that allows it. Further, this procedure can easily be continued to encompass more than two states.

3 Sample results

In this section, we shall illustrate the advantages of our schemes. First, we focus attention on a known problem (5), use various $\bar{\chi}$ in (8) to construct (10) that would satisfy (9). Section 3.1 will be devoted to such problems. Secondly, we shall employ known results of (5) and (6) to construct (22), the RE corresponding to (3), and discuss some of its consequences. This part will be addressed in Sect. 3.2 As known starting points, we consider the well known harmonic oscillator (HO) problem and the S-state Hamiltonian of the H-atom (HA) problem, after making an appropriate reduction [$R(r) = \Psi(r)/r, \Psi(r) \equiv \Psi(x)$].

3.1 Isoergic states

(i) We choose the $n = 0$ state of the HO that shows [see (5)]

$$\chi_{00} = -x, \quad \varepsilon_{00} = 1, \quad V_0 = x^2. \tag{23}$$

Let us take a simple form for $\bar{\chi}$:

$$\bar{\chi} = \frac{\alpha}{x} + \beta x^M. \tag{24}$$

The potential then becomes

$$V = \frac{\alpha(\alpha - 1)}{x^2} - 2\alpha + x^2 + \beta(2\alpha + M)x^{M-1} - 2\beta x^{M+1} + \beta^2 x^{2M}. \tag{25}$$

This V shows a lot of interesting features. For $\alpha \neq 0$ and $\alpha \neq 1$, the first term reveals a stronger singularity at the origin, while $M > 1$ shows a stronger singularity near the boundaries, relative to the parent potential. Bound states require that $\beta < 0$ and M odd. The special choice of $M = 3$ and $\alpha = 0$ was considered earlier. An interesting special case arises when we choose $\beta = 0$ and

$$\alpha(\alpha - 1) = \lambda, \quad \lambda > 0. \tag{26}$$

In this situation, the potential (25) would reduce to

$$V = \frac{\lambda}{x^2} - 2\alpha + x^2 \tag{27}$$

showing a repulsive core around $x = 0$. However, (26) yields a pair of α -values and the acceptable value that respects (27) will be

$$\alpha = \frac{1 + \sqrt{1 + 4\lambda}}{2}. \tag{28}$$

This is one typical example of spiked oscillators that have attracted considerable recent attention for varying reasons [18–23].

Obviously, innumerable examples would follow from the above route by considering different polynomial forms for $\bar{\chi}$ in (24).

(ii) We choose next the $n = 1$ state of the HO to note that terms in (5) are

$$\chi_{10} = \frac{1}{x} - x, \quad \varepsilon_{10} = 3, \quad V_0 = x^2. \quad (29)$$

The choice (24) for $\bar{\chi}$ is made again to obtain

$$V = \frac{\alpha(\alpha + 1)}{x^2} - 2\alpha + x^2 + \beta(2\alpha + M + 2)x^{M-1} - 2\beta x^{M+1} + \beta^2 x^{2M}. \quad (30)$$

For $\alpha = 0$, the potential (30) leads to the $n = 1$ state of (6). But, if $\alpha = -1$, we obtain the ground state of (6). In either case, however, we need to take $\beta < 0$ and M odd to ensure normalization of the wave function in $(-\infty, \infty)$. This example shows that the present recipe can connect states with different quantum numbers too.

(iii) Starting with the ground ($n = 1$) state of the HA, we identify the terms in (5) as

$$\chi_{10} = \frac{1}{x} - \frac{1}{2}, \quad \varepsilon_{10} = -\frac{1}{4}, \quad V_0 = -\frac{1}{x}. \quad (31)$$

The choice

$$\bar{\chi} = \alpha + \beta x \quad (32)$$

leads to the potential

$$V = \frac{2\alpha - 1}{x} + (\alpha^2 - \alpha + 3\beta) + (2\alpha - 1)\beta x + \beta^2 x^2. \quad (33)$$

Here, $\beta < 0$ is the proper choice and we note that (33) involves a special combination of spherical Stark and Zeeman effects [24–30] on a dressed HA. For $\alpha = 0$, identical effects on a pure HA is seen. The interesting part is that, all such potentials are solvable. A special choice of $\alpha = 1/2$ gives the spherical HO result.

(iv) As the final illustration of this subsection, we start from the $n = 2$ state of the HA, whereby terms in (5) look as follows:

$$\chi_{20} = \frac{1}{x} + \frac{1}{x-4} - \frac{1}{4}, \quad \varepsilon_{20} = -\frac{1}{16}, \quad V_0 = -\frac{1}{x}. \quad (34)$$

The first choice

$$\bar{\chi} = \alpha x \quad (35)$$

yields the potential

$$V = -\frac{1}{x} + \frac{2\alpha x}{x-4} + 3\alpha - \frac{\alpha x}{2} + \alpha^2 x^2 \quad (36)$$

corresponding again to mixed spherical Stark and Zeeman effects on a H-atom, but with an extra term that is singular at $x = 4$ to account for the excited state node. Our second choice is

$$\bar{\chi} = \alpha/(x-4) \quad (37)$$

leading to

$$V = -\frac{1}{x} \left(1 + \frac{\alpha}{2}\right) + \frac{\alpha(\alpha+1)}{(x-4)^2}. \quad (38)$$

The special choice of $\alpha = -1$ in (37) results in vanishing of the node at $x = 4$ and we get back effectively the 1s state. A related but more useful choice could be

$$\bar{\chi} = -\frac{1}{(x-4)} + \beta x \quad (39)$$

yielding

$$V = -\frac{1}{2x} + 3\beta - \frac{\beta x}{2} + \beta^2 x^2. \quad (40)$$

This potential again is a mixed perturbation result, like (33) or (36), but here on a scaled H-atom. One now experiences how various exactly solvable cases emerge from the above simple recipe.

3.2 States as products

- (i) We choose again the $n = 0$ state of the HO with the choice (23)

$$\chi_{00} = -x, \quad \varepsilon_{00} = 1, \quad V_0 = x^2 \quad (23)$$

and couple it with another solvable anharmonic potential system given by

$$\chi_0 = -x^3, \quad E_0 = 0, \quad V = x^6 - 3x^2. \quad (41)$$

The net result is

$$\chi_T = -x - x^3, \quad E_T = 1, \quad V_T = x^6 + 2x^4 - 2x^2. \quad (42)$$

This refers to the ground state of the potential V_T , accidentally here becomes isoergic with the HO ground state because $E_0 = 0$. Indeed, the outcome (42) agrees with (25) for $\alpha = 0$, $\beta = -1$ and $M = 3$.

- (ii) For the $n = 1$ state of the HO, we have the known set of results given by (29):

$$\chi_{10} = \frac{1}{x} - x, \quad \varepsilon_{10} = 3, \quad V_0 = x^2. \quad (29)$$

Coupled with (41), we obtain the $n = 1$ state with energy $E_T = 3$ for the potential

$$V_T = x^6 + 2x^4 - 4x^2, \quad (43)$$

which is identical with (30) for the choice $\alpha = 0$, $\beta = -1$ and $M = 3$. The reason is the same as that noted in (i).

- (iii) Consider now (31) and (34). Joining them as per rule, we see that

$$\chi_T = \frac{2}{x} + \frac{1}{x-4} - \frac{3}{4}, \quad E_T = -\frac{5}{16}, \quad V_T = \frac{2}{x^2} - \frac{4}{x} - \frac{1}{2(x-4)} + \frac{1}{4}. \quad (44)$$

This resembles a hydrogenic 3p-state barring that the node is not the natural one that arises out of orthogonality requirement; instead, it is due to an infinite point discontinuity in the potential at $x = 4$.

In order to see the emergence of a hydrogenic 2p-state with the same total energy as above (viz. $-5/16$), we need to additionally follow the approach outlined in 3.1. Choosing $\bar{\chi} = -1/(x-4)$ and considering (44) as the parent state, we recover the new targeted state of 2p-type defined by the potential

$$V = -\frac{3}{x} + \frac{1}{4} + \frac{2}{x^2}. \quad (45)$$

4 Further discussion

Apart from providing a clear and direct link among solvable states of the SE, which we achieve here by proceeding via a simpler route provided by the RE, the procedure outlined in Sect. 3.2 possesses a kinship with one more important idea, viz. the MME, as indicated earlier. We like to briefly discuss it here.

Let us first outline the spirit behind MME. Since exact solutions of the Schrödinger energy eigenvalue problem for bound states, defined by

$$H\Psi_n = E_n\Psi_n, \quad \langle \Psi_m | \Psi_n \rangle = \delta_{mn}, \quad (46)$$

are available only for a few systems, often approximate solutions of (1) are sought. The variational method offers a general route in this context. While for the ground state ($n = 0$), an unconstrained variation method works, the same is not true of excited ones, though, for states of lowest energies of a given symmetry, one can employ unconstrained variations provided the trial state possesses the specific symmetry information. In general, therefore, we proceed via a linear variational framework, particularly for excited-state calculations. The concept of manifold energy appears in the course of such a linear variational set up as follows. Suppose we choose an arbitrary N dimensional linear manifold spanned by a set of admissible functions $\{\theta_j\}$, $j = 0, 1, \dots, N - 1$, with $\langle \theta_j | \theta_k \rangle = \delta_{jk}$. We then define the manifold energy by $\varepsilon(N)$ where

$$\varepsilon(N) = \sum_{j=0}^{N-1} \langle \theta_j | H | \theta_j \rangle = \sum_{j=0}^{N-1} H_{jj}. \quad (47)$$

Particularly important is to notice the bound

$$\varepsilon(N) \geq E(N) \quad (48)$$

where the right side of (47) signifies the sum of first N exact energy-levels of (1), i.e.,

$$E(N) = \sum_{j=0}^{N-1} E_j. \quad (49)$$

It is on the basis of (48) that a variational method has been suggested, called the MME [6, 7]. The aim is to replace the age-old tradition of minimization of the ground-state energy (MGE)[31]. The MME has been advocated especially in MCSCF-type of calculations where bases θ_j contain one or more nonlinear parameters embedded in them. One can, therefore, pursue a coupled variational scheme. Symbolically, we write $\theta_j = \theta_j(\alpha)$. The quantity $\varepsilon(N)$ will then depend on α , and hence can be varied to obtain its minimum value. Such an approach has indeed turned out to be quite rewarding in excited-state calculations [32]. Let us note that (48) follows for any $K \leq N$. However, while MGE is apt for the best ground state at some given N , and excited states orthogonal to it emerge, the MME is believed to furnish a more balanced description of several states K at a time, where $K \leq N$.

Having realized that the concept of MME rests on a linear manifold, we proceed to note the following. It is apparent from (48) that, while $\varepsilon(N)$ depends both on the chosen linear manifold and H , the real bound is provided by $E(N)$ that is characteristic of H only. So, one may be tempted to enquire whether MME stands as a mere mathematical theorem in linear space or is linked with lowest energies of some suitable physical systems. Indeed, once such a system is found, we can talk of unconstrained variations for $E(N)$ as well, at any N , without referring to the MME, and then the method becomes more general and effective.

In linear variations, we define the matrix elements $H_{ij} = \langle \theta_i | H | \theta_j \rangle$, construct the $N \times N$ Hamiltonian matrix \mathbf{H} and diagonalize it to obtain N eigenvalues.

These are ordered as $\bar{\varepsilon}_0(N) \leq \bar{\varepsilon}_1(N) \leq \bar{\varepsilon}_2(N) \dots$ etc. The corresponding eigenvectors are labeled as $\bar{\theta}_0(N)$, $\bar{\theta}_1(N)$, $\bar{\theta}_2(N)$, \dots etc. One can then show the following results [33,34]:

$$E_k \leq \bar{\varepsilon}_k(N+1) \leq \bar{\varepsilon}_k(N), \quad k = 0, 1, 2, \dots \quad (50)$$

$$\langle \bar{\theta}_j | \bar{\theta}_k \rangle = \delta_{jk}; \quad \langle \bar{\theta}_j | H | \bar{\theta}_k \rangle = \bar{\varepsilon}_k \delta_{jk}. \quad (51)$$

In view of (50), inequality (48) follows, and it forms the basis of the MME, remembering that the quantity at the left of (48) refers to the trace that remains invariant in going from $\theta_j \rightarrow \bar{\theta}_j$. One also finds from (50) that (48) would follow for any $K \leq N$ as well. Further, if elements of the set $\{\theta_j\}$ contain one or more nonlinear parameters that we symbolize by $\theta_j = \theta_j(\alpha)$, the above conclusions remain true at each α and hence at the optimum α chosen to minimize the left side of (48). Here lies the strength of the MME. Usually, however, one chooses α to minimize $\bar{\varepsilon}_0(N)$, and this corresponds to the MGE.

To establish the aforesaid kinship, we designate the SUSY partner potential of V_0 in (1) by V_1 and call the resultant Hamiltonian by H_1 that satisfies

$$H_1 \Psi_{n1} = E_{n1} \Psi_{n1}. \quad (52)$$

For convenience, we call $\varepsilon_{n0} = E_{n0}$. The RE corresponding to (52) becomes

$$\chi_{n1}^2 + \chi'_{n1} + E_{n1} - V_1 = 0. \quad (53)$$

The process continues by defining V_2 as the SUSY partner of V_1 with the SE

$$H_2 \Psi_{n2} = E_{n2} \Psi_{n2}, \quad (54)$$

for which the RE reads as

$$\chi_{n2}^2 + \chi'_{n2} + E_{n2} - V_2 = 0. \quad (55)$$

In all such cases, the ground state is defined by $n = 0$. We then have

$$E_{10} = E_{01}, \quad E_{20} = E_{11} = E_{02}, \quad (56)$$

etc. by virtue of the properties of SUSY partner potentials. Now, we are in a position to generate the tailor-made systems. Adding (5) and (53) for the $n = 0$ state, we find

$$(\chi_{00}^2 + \chi_{01}^2) + (\chi'_{00} + \chi'_{01}) + (E_{00} + E_{01}) - (V_0 + V_1) = 0. \quad (57)$$

A rearrangement yields

$$(\chi_{00} + \chi_{01})^2 + (\chi_{00} + \chi_{01})' + (E_{00} + E_{01}) - (V_0 + V_1 + 2\chi_{00}\chi_{01}) = 0. \quad (58)$$

Note that (58) is a special case of (20); here the only restriction is that the χ functions considered refer to ground states. An equation like (58) shows the potential for which the ground state energy appears as a sum of the ground and first excited states of the parent potential V_0 . This procedure can be continued to involve three or more states easily and hence MME finds significance in terms of an unconstrained variational route that is characteristic of the MGE. In fact, our earlier example (45) showed already a way of achieving the same end without reference to SUSY. However, for problems that are not exactly solvable, one has to construct the cross χ terms in potentials approximately. Then, the upper bound property of MGE will be lost, though one can approach exactness as the χ terms improve in quality.

5 Conclusion

In summary, our primary endeavor has been to find solvable states with pre-assigned energies in specified potential fields. We have found that, it is expedient to proceed via the RE in place of the SE to achieve this end and devised two such routes. The link of one such strategy with SUSY quantum mechanics is established. We have also outlined how the other route is linked with MME in a variational context. While this work is focused on finding exact solutions, we have, in fine, indicated how the recipe can be extended for approximate calculations as well. Future work along this direction would justify the efficacy of the procedure. Of particular concern in one such context may be to explore how the SUSY-inspired WKB scheme [35–37] would fare for potentials leading to specific isoergic states.

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