

A simple and effective technique to variationally interpret the structure of SUSY partners of mirror image potentials

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Abstract Precise supersymmetric partner potentials can be generated for exactly solvable problems of the stationary Schrödinger equation. Construction of isospectral potential is not always possible for exactly solvable systems. This is a restriction, as most problems are not exactly solvable. Employment of mirror-image property can help to construct an exact isospectral partner of that potential. These potentials have chemical relevance to enantiomers. In this paper, we present a formulation as modelling to explore the form of SUSY pair of these potentials. Through polynomial fit, we correlate all possible basic SUSY partners and optimise it to best fit polynomial to present a typical energy value of $N=50$.

Keywords SUSY quantum mechanics · Mirror image potentials · Isospectrality · Enantiomers

1 Introduction

Resurgence in studies of exactly solvable Hamiltonians has taken place with the advent of supersymmetric (SUSY) quantum mechanics [1–23]. After some early work [1], links among SUSY, factorization method and Darboux transformation have been highlighted in the literature [2–5]. One of the most important concepts is the construction isospectral potentials [24]. But curiously, most of the potentials in quantum mechanics are not exactly solvable, and one has to employ variation principle [25,26] or perturbation theory [27] to calculate their approximate wave function as well as energy. Thus barring few potentials, it is impossible to construct their isospectral partner potentials. In this context, mirror image property has been employed to construct the

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isospectral partner potential of asymmetric potentials. In chemistry, isospectral potentials have significant importance but yet not been extensively studied. One can expect this isospectrality especially in nanostructures [28] and charge transfer complexes. Even molecules having same number of electron can have identical spectrum [29–31]. Secondly, mirror image property is a well known concept in chemistry. In stereochemistry enantiomers [32] are well known. Pair of molecules having non-superimposable mirror image structure is called enantiomer. These Enantiomers are two different molecules having same chemical formula but different structure, as a result have different chemical and physical properties but identical energy. Depending upon their optical properties i.e. how the pair of molecules respond to a plane polarized light they are termed as dextro (*d*) (positive optical rotation meaning clockwise) and levo (*l*) (negative optical rotation meaning anticlockwise). Thus enantiomer is termed as *d-l* pair. The most common example of such enantiomers is D-glucose and L-glucose. But D-glucose is only naturally occurring and L-glucose has to be artificially synthesized. But it is also not known how their potentials are related. Then also have same optical activity in magnitude but in opposite directions. In this endeavour our aim is to formulate 1D model to enantiomers. Then we try to construct the SUSY partner of these model potentials. The potentials related by mirror image have same energy spectrum and thereby one can assume how potentials of enantiomers are related in appreciation of their physico-chemical properties. To illustrate this phenomena on the theoretical perspective, property based studies are also elaborated.

2 Concepts and objectives

Isospectrality is a concept where the potentials of different chemical or physical environment have identical energy spectrum. Let us take two isospectral potentials $V_1(x)$ and $V_2(x)$. $V_1(x)$ and $V_2(x)$ are related as

$$V_1(x) = V_2(x) + f(x) \quad (1)$$

Because of the fact that $V_1(x)$ and $V_2(x)$ are isospectral, it can be said that if one applies a perturbation of $f(x)$ on $V_2(x)$, this perturbation will only change its eigen functions but not their eigen values. Thus if one knows the eigen function and eigen value of $V_2(x)$, then by applying perturbation theory he can easily get the information about the eigen states of these potentials. Although $V_1(x)$ and $V_2(x)$ have same energy spectrum but one must get energy correction term during perturbative calculations. This is because in Raleigh-Schrödinger perturbation theory [27] to get wave correction term one needs to know the energy correction term of previous order. This is indeed an interesting problem. There is a route to construct isospectral partner potential using SUSY theory [24].

Let us consider a potential $V_0(x)$ with ground state normalised eigen function $\psi_0(x)$ and energy E_0 . Then applying the conventional SUSY theory one can easily construct its SUSY partner $V_3(x)$ as follows;

$$V_3(x) = V_0(x) - 2 \frac{d^2}{dx^2} \ln \psi_0 \quad (2)$$

The energies of $V_0(x)$ and $V_3(x)$ are related as

$$E_n^3 = E_{n+1}^0 \quad n = 0, 1, 2, \dots \quad (2a)$$

The energy eigen state E_0 vanishes for potential $V_3(x)$. But the function $\left(\frac{1}{\psi_0(x)}\right)$ satisfies the Schrödinger equation with $V_3(x)$ and energy E_0 . One can construct more linearly independent solutions for the same state like $\frac{\int_{-\infty}^x \psi_i^2(x') dx'}{\psi_0(x)}$ and the most general solution of the Schrödinger equation with $V_3(x)$ and energy E_0 is $\Psi_0(x, \lambda_0) = \frac{\int_{-\infty}^x \psi_i^2(x') dx' + \lambda_0}{\psi_0(x)}$, where λ_0 is a real constant which does not have value in the range $-1 \leq \lambda_0 \leq 0$. This is because the value of integral part in the numerator varies between 0 to 1. Thus there is always a possibility of vanishing of wave function $\Psi_0(x, \lambda_0)$ in the finite range.

Finally, employing the SUSY procedure [1–23], one can add that state E_0 to a potential

$$\hat{V}_0(x, \lambda_0) = V_3(x) - 2 \frac{d^2}{dx^2} \ln[\Psi_0(x, \lambda_0)] \quad (3)$$

Now, $V_0(x)$ and $\hat{V}_0(x)$ are two isospectral partners having same SUSY partner $V_3(x)$. These isospectral partners related as from Eqs. (2) and (3),

$$\hat{V}_0(x, \lambda_0) = V_0(x) - 2 \frac{d^2}{dx^2} \ln[\psi_0(x) \Psi_0(x, \lambda_0)] \quad (4)$$

These are one parameter family of isospectral potential. Now, one can construct n-parameter family of isospectral potential using the same theory. Then isospectral potential and the parent potential have the common nth SUSY partner. Having the following form

$$\hat{V}_0(x, \lambda_0 \dots \lambda_{n-1}) = V_0(x) - 2 \frac{d^2}{dx^2} \ln[\psi_0 \psi_1 \dots \psi_{n-1} \Psi_{n-1}(x, \lambda_{n-1}) \dots \Psi_0(x, \lambda_0, \lambda_1 \dots, \lambda_{n-1})] \quad (5)$$

The $\frac{1}{\psi_i}$ in Eq. (5) represents the Eigen functions of $\hat{V}_0(x, \lambda_0 \dots \lambda_{n-1})$.

Thus to construct the n-parameter isospectral partner, one needs to know the exact wave function of the parent potential up to (n–1)th excited state. But the problems are more severe. Firstly, in quantum mechanics most of the potential are not exactly solvable. Even ground states are not exactly known. Moreover the integral part in all $\Psi_i(x)$ is difficult to solve. Even in the case of harmonic oscillator, the integral results error function ($erfc(x')$) [33]. This is a severe restriction in construction of precise isospectral partner potentials. Secondly in this theory the parent potential and the isospectral partner have at least one common SUSY partner.

Thus simple and effective way out is that to focus on the property, structure and nature of parent potential, and then use those concepts to construct the isospectral partner. The easiest way is to construct their mirror image partner potential and analyse

them. Another objective is to know how the SUSY partners of these two mirror image pair related. In this paper, first we construct the isospectral partner potential of a given asymmetric potential using mirror image property. Then we try to relate them with enantiomers and construct their SUSY partner in precise form. Finally we analyse the SUSY partners. The study of some useful properties of these pair of potentials is also interesting. These types of mirror image potentials have special interests in chemistry as well as physics. In case of symmetric potentials, there is parity. In asymmetric potentials ($-\infty \leq V(x) \leq \infty$), we always get such mirror image pair. Anharmonic oscillator potentials are always in the centre of interest. Many theories in chemistry and physics are explained using these types of potentials. One needs to choose anharmonic potentials to study quantum chemistry in 1-D model calculations. Even these model potentials are the most physical approximation to the molecular system in 1-Dimension. Thus any theory or demonstration involving anharmonic oscillator potentials have immense physical importance. Here, the potentials of our interest are also anharmonic one.

In this context coupled variation scheme is employed to study the lower energy states (0–19), construct the near-exact SUSY partner potential of these pair potentials. Wilson-Sommerfeld quantisation rule [34] is applied for higher excited states of SUSY partner to verify the mirror image property of the constructed SUSY partner potentials.

The organization is as follows. Section 3, will concentrate on formalism. Section 4 will inform about the strategy and trial states. Pilot calculations to demonstrate the basic methods with its various variants will concern us in Sect. 5. Section 6, contains summarization of the major conclusions of these formulation.

3 Formalism

The generalised form of the potential of present interest,

$$V(x) = \sum_{m=2}^k a_m x^m + \sum_{n=1}^l b_n x^n \quad (6)$$

where, m is even and n is odd, also for bound potential $k > 1$.

These type of potentials consist of symmetric and asymmetric terms and depending upon the value of $|b_n|$ we always get mirror image potential pair. The highest power of x - in these type of potentials must be even and the coefficient with that term also must be positive. Moreover with increase of the symmetric and asymmetric terms in $V(x)$, number of such pair increases. Actually if one replace x by $-x$ in one potential of this form, he will obviously get the other one. The wave function changes according to the potential. Change of co-ordinate will not change the energy. We expect these mirror image potential to be isospectral. These potentials have asymmetric properties of same magnitude with opposite sign. This explains the opposite optical rotation of the enantiomers. The effect of any asymmetric perturbation is different in these types of potentials. This point is similar to the different reactivity of enantiomers towards same reagents.

In this work, as one of the objectives is to verify the mirror image property of the SUSY partner potentials. Theoretically by employing the variation method it is possible to calculate the lower excited state. But in higher excited state it is very difficult to use. Because computation become more costly and time consuming. Even in case of SUSY partners, where there potential form is not compact. Calculation using conventional variational theory is practically impossible. Thus in this context, we employ Wilson-Sommerfeld quantisation rule to calculate the higher energy states like $n = 1,000$ or more,

$$\int_{x_2}^{x_1} \sqrt{E_n - V(x)} dx = n\hbar \quad (7)$$

here, x_1, x_2 are the left and right boundary of the classical limits. Using this Eq. (7), we will not be able to get the semiclassical energy of the desire state. But using this we can easily compare the higher excited state of two potential expected to be isospectral. Suitable match of the SUSY partners can also be verified. Application of this rule will, qualitatively, serve the purpose. If the energy states obtained by using both the potential are same then one can't say that the pair is mirror image. Thus we have derived Best fit polynomial expression to the SUSY partners. If these derived one follows the Eq. (6) then they are mirror image. The steps can be pointed as:

- We calculate the ground and lower excited state energies of the SUSY partner potential using coupled variation principle.
- We calculate the higher excited state energy of the SUSY partner potential using Wilson-Sommerfeld quantisation rule.
- Then we compare the E_n of both the potentials. In all cases they must be equal and
- We finally optimise the best fit polynomial to the SUSY partners. Then we verify them by using variation principle and Eq. (6).

4 The strategy

The first aim is to construct the SUSY partner potentials. Recently considerable work is reported in respect of successful construction of the best possible SUSY partners $\bar{V}_0^+(x)$ using both linear and non-linear variation techniques [35,36]. This construction can easily been explained by variation concept, by increasing the parameter in the trial function we can increase the accuracy of the result. More accurate the result is more accurate will be the SUSY partner. Thus one has to employ the equation

$$V_0^+(x) = V_0(x) - 2 \frac{d^2}{dx^2} \ln \bar{\psi}_0 \quad (8)$$

Finally, it will be checked whether

$$\Delta T_P^2 = \Delta V_P^2 = \Delta T_I^2 = \Delta V_I^2 \quad (9)$$

(here, P is for parent potential and I is for its isospectral partner) is true for this mirror image isospectral pair. Actually one of the necessary conditions of a bound stationary state to obey is

$$\Delta T_n^2 = \Delta V_n^2 \quad (10)$$

This is a virial like theorem. Recently, these necessary conditions have been employed to optimise the stationary state [37].

Practical success of the above-mentioned strategy depends crucially on the well behave nature of wave function. The general feature of the variational method is that the energy is more accurately obtained than the wave function. In our case, however, accuracy of the wave function is of prime importance. Therefore, near-exact ψ_0 is required. An additional point is that the low lying average energies, convergence of which dictates the goodness of the corresponding wave functions mentioned above in linear variations, take proper account of the potential only around a small region of the origin and not the effect of the potential at large distances. Hence, unless one goes for higher-energy calculations with Eq. (6), it is difficult to say whether the generated SUSY partners are really precise. So, one needs to examine how accurately a few high-energy levels are estimated via this formalism. Thus, polynomial curve fitting has been applied to get the precise form of SUSY partners. Then these precise SUSY partner potentials are diagonalised to check how good they are. In this case same is also true that with increase of N goodness of ψ increases and also the correctness of the SUSY partners.

The final part is the proper choice of basis functions. Here, we choose to employ the Hermite polynomial (H_i) along with their weight factor as basis function. These bases have already been found to be quite convenient in several types of variational calculations. They possess nice convergence properties as well. The trial state has the form,

$$\tilde{\psi}_n = \sum_{i=0}^N c_{in} H_i(x, a) \exp(-ax^2) \quad (11)$$

The virtues of using such basis functions are, in brief, as follows. First, integrals involved in \mathbf{H} are quite easy to evaluate. Second, existence of the nonlinear variational parameter ‘ a ’ allows one to adopt a coupled variational scheme that is far more powerful than purely linear variations. Third, convergence of the process as a function of N is ensured. Note that the basis set leads ultimately to a secular equation at each a . But, we also realize that the potential energy part becomes infinitely large as $a \rightarrow 0$. At the other extreme, when $a \rightarrow \infty$, the kinetic energy part behaves in a similar fashion. Thus, qualitatively, the uncertainty principle guarantees the existence of an optimal choice for ‘ a ’. So, the practice is to adopt the following scheme. One choose a trial value for ‘ a ’, constructs the \mathbf{H} matrix, diagonalises it, and optimize the coefficients such that the lowest energy is minimized, then one has to continue the same process at other a -values, and finally pick out the minimum of all such minima, corresponding to the optimal a -value. The states and energies are then assigned according to the usual practice of linear variation.

The tasks are now in order. Initially we solve the secular equation obtained by the coupled variation scheme for the pair of mirror image potential to know the energy spectrum and near-exact SUSY partner of them. Then we employ coupled variation scheme and the Wilson-Sommerfeld quantisation rule to check the energy states of the SUSY partner potential. Finally we verify the mirror image property using polynomial fitting.

5 Result and discussion

In this calculation four mirror image pair of potentials has been selected for study. They are,

- I) Pair 1: $V_1(x) = x^4 + x^3$
 $V_2(x) = x^4 - x^3$
- II) Pair 2: $V_3(x) = x^2 + 3x$
 $V_4(x) = x^2 - 3x$
- III) Pair 3: $V_5(x) = x^6 + 5x^3$
 $V_6(x) = x^6 - 5x^3$
- IV) Pair 4: $V_7(x) = x^8 + 8x^3$
 $V_8(x) = x^8 - 8x^3$

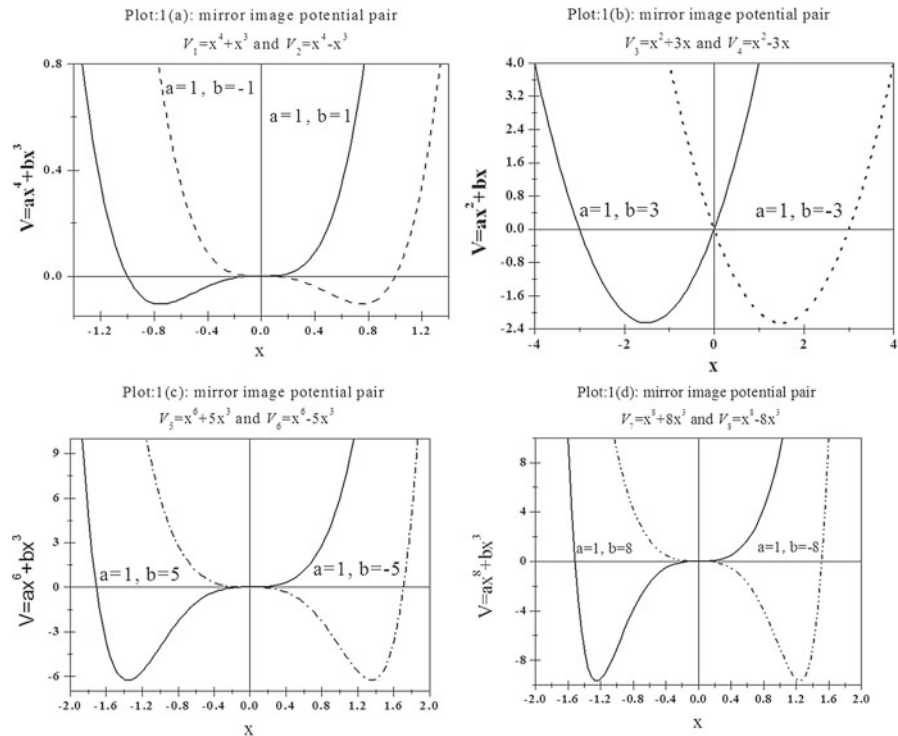


Fig. 1 Isospectral mirror image partner potential (pair: 1–4)

Table 1 Variational upper bound energies of potential $V_1 (\bar{E}_n(V_1))$ and $V_2 (\bar{E}_n(V_2))$ to show their Isospectrality and the energies of the constructed SUSY partners of $V_1 (\bar{E}_n(V_1^+))$ and $V_2 (\bar{E}_n(V_2^+))$

n	$\bar{E}_n(V_1)$	$\bar{E}_n(V_2)$	$\bar{E}_n(V_1^+)$	$\bar{E}_n(V_2^+)$
0	0.905 341 223 793 293 28	0.905 341 223 793 293 28	3.441 398 835 169 418 79	3.441 398 835 169 418 79
1	3.441 398 835 169 418 88	3.441 398 835 169 418 88	6.970 309 110 900 634 05	6.970 309 110 900 634 05
2	6.970 309 110 900 634 21	6.970 309 110 900 634 21	11.041 884 907 548 959 57	11.041 884 907 548 959 57
3	11.041 884 907 548 959 97	11.041 884 907 548 959 97	15.552 647 608 481 105 20	15.552 647 608 481 105 20
4	15.552 647 608 481 105 80	15.552 647 608 481 105 80	20.430 458 513 628 287 45	20.430 458 513 628 287 45
5	20.430 458 513 628 288 23	20.430 458 513 628 288 23	25.627 639 475 436 256 25	25.627 639 475 436 256 25
6	25.627 639 475 436 257 23	25.627 639 475 436 257 23	31.109 500 173 010 151 19	31.109 500 173 010 151 19
7	31.109 500 173 010 151 19	31.109 500 173 010 151 19	36.849 478 931 821 458 95	36.849 478 931 821 457 35
8	36.849 478 931 821 458 95	36.849 478 931 821 458 95	42.826 460 929 066 198 44	42.826 460 929 066 196 60
9	42.826 460 929 066 198 44	42.826 460 929 066 198 44	49.023 183 035 279 660 65	49.023 183 035 279 658 45
10	49.023 183 035 279 660 65	49.023 183 035 279 660 65	55.425 218 586 210 734 27	55.425 218 586 210 731 75
11	55.425 218 586 210 734 27	55.425 218 586 210 734 27	62.020 297 591 051 758 62	62.020 297 591 051 755 87
12	62.020 297 591 051 758 62	62.020 297 591 051 758 62	68.797 832 783 068 592 70	68.797 832 783 068 589 10
13	68.797 832 783 068 592 70	68.797 832 783 068 592 70	75.748 578 140 791 530 19	75.748 578 140 791 526 34
14	75.748 578 140 791 530 19	75.748 578 140 791 530 19	82.864 376 044 604 511 90	82.864 376 044 604 505 21
15	82.864 376 044 604 511 90	82.864 376 044 604 511 90	90.137 965 697 127 776 71	90.137 965 697 127 768 97
16	90.137 965 697 127 776 71	90.137 965 697 127 776 71	97.562 835 071 086 141 30	97.562 835 071 086 135 29
17	97.562 835 071 086 141 30	97.562 835 071 086 141 30	105.133 104 523 771 768 2	105.133 104 523 771 587 9
18	105.133 104 523 771 768 2	105.133 104 523 771 768 2	112.843 433 927 803 154 8	112.843 433 927 803 021 5
19	112.843 433 927 803 154 8	112.843 433 927 803 154 8		

Table 2 Variational upper bound energies of potential V_3 ($\bar{E}_n(V_3)$) and V_4 ($\bar{E}_n(V_4)$) to show their Isospectrality and the energies of the constructed SUSY partners of V_3 ($\bar{E}_n(V_3^+)$) and V_4 ($\bar{E}_n(V_4^+)$)

n	$\bar{E}_n(V_3)$	$\bar{E}_n(V_4)$	$\bar{E}_n(V_3^+)$	$\bar{E}_n(V_4^+)$
0	-1.250	-1.250	0.750 000 000 000 000 20	0.750 000 000 000 000 20
1	0.750	0.750	2.750 000 000 000 000 95	2.750 000 000 000 000 95
2	2.750	2.750	4.750 000 000 000 001 25	4.750 000 000 000 001 25
3	4.750	4.750	6.750 000 000 000 001 65	6.750 000 000 000 001 65
4	6.750	6.750	8.750 000 000 000 002 79	8.750 000 000 000 002 79
5	8.750	8.750	10.750 000 000 000 003 58	10.750 000 000 000 003 58
6	10.750	10.750	12.750 000 000 000 004 97	12.750 000 000 000 004 97
7	12.750	12.750	14.750 000 000 000 006 10	14.750 000 000 000 006 10
8	14.750	14.750	16.750 000 000 000 006 76	16.750 000 000 000 006 76
9	16.750	16.750	18.750 000 000 000 007 46	18.750 000 000 000 007 46
10	18.750	18.750	20.750 000 000 000 008 27	20.750 000 000 000 008 27
11	20.750	20.750	22.750 000 000 000 009 11	22.750 000 000 000 009 11
12	22.750	22.750	24.750 000 000 000 009 78	24.750 000 000 000 009 78
13	24.750	24.750	26.750 000 000 000 010 43	26.750 000 000 000 010 43
14	26.750	26.750	28.750 000 000 000 010 78	28.750 000 000 000 010 78
15	28.750	28.750	30.750 000 000 000 011 28	30.750 000 000 000 011 28
16	30.750	30.750	32.750 000 000 000 011 78	32.750 000 000 000 011 78
17	32.750	32.750	34.750 000 000 000 012 56	34.750 000 000 000 012 56
18	34.750	34.750	36.750 000 000 000 012 78	36.750 000 000 000 012 78
19	36.750	36.750		

Figure 1 shows how these four pairs are individually related. The members of each pair are mirror images to each other. All the eight potentials are familiar anharmonic oscillator models with one symmetric and other asymmetric term. Construction of mirror image potential is easy. If one changes the sign of the co-efficient of asymmetric term in a bound potential, he obtains the mirror image pair of that potential. Let us initiate the discussion by checking the energies of the various processes. Theoretically each of the above pair is isospectral. Here, quantitatively energy description is necessary to analyse the SUSY partner potential and their mirror image property as well as isospectrality. The partner potential Equation in (8) is constructed a priori through the variational method applied on Eq. (2) by using Eq. (8). The Tables 1, 2, 3 and 4 would not only ensure the Isospectrality in lower energy states for all these constructed SUSY partners but also helps in analysing them. A glance at the 4th and 5th columns of Tables 1, 2, 3 and 4 reveals how nicely both the schemes converge. Only, we observe slight departures, at any fixed N, between the parent and SUSY partner potential. But, this is not surprising because here near-exact SUSY partner constructed. Here, for demonstrative purposes, we restrict ourselves up to N=50. But, one needs to go beyond to obtain good results for higher excited states. This can be achieved by routinely increasing the size N of the **H** matrix.

Table 3 Variational upper bound energies of potential $V_5 (\bar{E}_n(V_5))$ and $V_6 (\bar{E}_n(V_6))$ to show their Isospectrality and the energies of the constructed SUSY partners of $V_5 (\bar{E}_n(V_5^+))$ and $V_6 (\bar{E}_n(V_6^+))$

n	$(\bar{E}_n(V_5))$	$(\bar{E}_n(V_6))$	$(\bar{E}_n(V_5^+))$	$(\bar{E}_n(V_6^+))$
0	-1.698 601 384 859 746 33	-1.698 601 384 859 746 33	2.479 760 625 120 981 53	2.479 760 625 120 981 53
1	2.479 760 625 120 981 62	2.479 760 625 120 981 62	7.096 343 069 546 908 62	7.096 343 069 546 908 62
2	7.096 343 069 546 908 86	7.096 343 069 546 908 86	12.901 707 906 356 940 16	12.901 707 906 356 940 16
3	12.901 707 906 356 940 45	12.901 707 906 356 940 45	19.666 943 469 561 410 52	19.666 943 469 561 410 52
4	19.666 943 469 561 411 04	19.666 943 469 561 411 04	27.243 441 245 545 072 79	27.243 441 245 545 071 24
5	27.243 441 245 545 072 79	27.243 441 245 545 072 79	35.551 119 271 798 073 91	35.551 119 271 798 072 21
6	35.551 119 271 798 073 91	35.551 119 271 798 073 91	44.529 308 516 268 471 71	44.529 308 516 268 469 61
7	44.529 308 516 268 471 71	44.529 308 516 268 471 71	54.130 554 043 592 220 65	54.130 554 043 592 218 63
8	54.130 554 043 592 220 65	54.130 554 043 592 220 65	64.316 397 510 091 462 81	64.316 397 510 091 460 36
9	64.316 397 510 091 462 81	64.316 397 510 091 462 81	75.054 801 005 858 447 84	75.054 801 005 858 445 22
10	75.054 801 005 858 447 84	75.054 801 005 858 447 84	86.318 520 003 931 041 86	86.318 520 003 931 038 82
11	86.318 520 003 931 041 86	86.318 520 003 931 041 86	98.084 006 353 192 886 84	98.084 006 353 192 883 62
12	98.084 006 353 192 886 84	98.084 006 353 192 886 84	110.330 636 035 423 576 38	110.330 636 035 423 573 09
13	110.330 636 035 423 576 38	110.330 636 035 423 576 38	123.040 146 855 988 472 47	123.040 146 855 988 467 65
14	123.040 146 855 988 472 47	123.040 146 855 988 472 47	136.196 217 527 403 378 23	136.196 217 527 403 372 45
15	136.196 217 527 403 378 23	136.196 217 527 403 378 23	149.784 145 262 425 632 07	149.784 145 262 425 624 17
16	149.784 145 262 425 632 07	149.784 145 262 425 632 07	163.790 593 963 346 091 16	163.790 593 963 346 081 13
17	163.790 593 963 346 091 16	163.790 593 963 346 091 16	178.203 394 228 610 455 64	178.203 394 228 610 445 08
18	178.203 394 228 610 455 64	178.203 394 228 610 455 64	193.011 382 184 289 628 55	193.011 382 184 289 615 14
19	193.011 382 184 289 628 55	193.011 382 184 289 628 55		

Table 4 Variational upper bound energies of potential V_7 ($\bar{E}_n(V_7)$) and V_8 ($\bar{E}_n(V_8)$) to show their Isospectrality and the energies of the constructed SUSY partners of V_7 ($\bar{E}_n(V_7^+)$) and V_8 ($\bar{E}_n(V_8^+)$)

n	$(\bar{E}_n(V_7))$	$(\bar{E}_n(V_8))$	$(\bar{E}_n(V_7^+))$	$(\bar{E}_n(V_8^+))$
0	-2.668 804 706 984 087 880	-2.668 804 706 984 087 880	2.920 841 171 472 823 013	2.920 841 171 472 823 013
1	2.920 841 171 472 823 290	2.920 841 171 472 823 290	8.664 266 367 646 561 248	8.664 266 367 646 561 248
2	8.664 266 367 646 561 660	8.664 266 367 646 561 660	15.948 240 970 472 814 7	15.948 240 970 472 814 7
3	15.948 240 970 472 817 0	15.948 240 970 472 817 0	24.551 410 742 739 670 1	24.551 410 742 739 670 1
4	24.551 410 742 739 673 2	24.551 410 742 739 673 2	34.339 188 428 078 311 9	34.339 188 428 078 311 9
5	34.339 188 428 078 316 0	34.339 188 428 078 316 0	45.229 887 356 370 032 3	45.229 887 356 370 032 3
6	45.229 887 356 370 035 5	45.229 887 356 370 035 5	57.157 539 161 794 612 7	57.157 539 161 794 612 7
7	57.157 539 161 794 616 7	57.157 539 161 794 616 7	70.067 386 252 631 152 4	70.067 386 252 631 148 5
8	70.067 386 252 631 152 4	70.067 386 252 631 152 4	83.913 257 955 370 639 2	83.913 257 955 370 618 6
9	83.913 257 955 370 639 2	83.913 257 955 370 639 2	98.655 602 620 448 462 4	98.655 602 620 448 410 4
10	98.655 602 620 448 462 4	98.655 602 620 448 462 4	114.260 055 508 157 762	114.260 055 508 157 26 1
11	114.260 055 508 157 762	114.260 055 508 157 762	130.696 394 447 228 499	130.696 394 447 227 991
12	130.696 394 447 228 499	130.696 394 447 228 499	147.937 764 028 734 278	147.937 764 028 733 562
13	147.937 764 028 734 278	147.937 764 028 734 278	165.960 087 513 238 194	165.960 087 513 237 671
14	165.960 087 513 238 194	165.960 087 513 238 194	184.741 612 607 324 754	184.741 612 607 323 603
15	184.741 612 607 324 754	184.741 612 607 324 754	204.262 554 676 396 093	204.262 554 676 395 181
16	204.262 554 676 396 093	204.262 554 676 396 093	224.504 812 237 800 082	224.504 812 237 798 159
17	224.504 812 237 800 082	224.504 812 237 800 082	245.451 737 014 314 630	245.451 737 014 312 927
18	245.451 737 014 314 630	245.451 737 014 314 630	267.087 945 828 326 610	267.087 945 828 324 789
19	267.087 945 828 326 610	267.087 945 828 326 610		

Table 5 Higher excited state energy calculation of the SUSY partner potentials of potential pair 1 to verify their mirror image property and Isospectrality using Wilson-Sommerfeld Quantisation Rule

n	\bar{E}_n of the parent isospectral pair	$\bar{E}_n(V_1^+)$	$\bar{E}_n(V_2^+)$
24		399.039 478 273 750 390 20	399.039 478 273 750 390 20
25	399.039 478 273 750 391 24		
49		1008.745 583 883 673 318 39	1008.745 583 883 673 318 39
50	1008.745 583 883 673 315 21		
99		2546.995 078 290 921 169 04	2546.995 078 290 921 169 04
100	2546.995 078 290 921 168 51		
199		6426.125 496 071 596 302 5	6426.125 496 071 596 302 5
200	6426.125 496 071 596 304 50		
499		21825.362 624 324 871 407 1	21825.362 624 324 871 407 1
500	21825.362 624 324 871 408 01		
999		55020.097 040 901 259 755 1	55020.097 040 901 259 755 1
1000	55020.097 040 901 259 756 1		
1999		138679.518 730 994 970 240	138679.518 730 994 970 240
2000	138679.518 730 994 970 23 4		
4999		470641.488 076 347 255 450	470641.488 076 347 255 450
5000	470641.488 076 347 255 43 2		
9999		1186054.416 214 502 646 60	1186054.416 214 502 646 60
10000	1186054.416 214 502 646 13		
49999		10141651.959 707 772 500	10141651.959 707 772 500
50000	10141651.959 707 772 300		
99999		25555866.013 245 017 565 5	25555866.013 245 017 565 5
100000	25555866.013 245 017 545 2		

Our focus is on the SUSY partners of these isospectral mirror image pairs. Then employing the Wilson-Sommerfeld quantisation rule (Tables 5, 6, 7, 8) we can easily check the equality of the energies of the higher excited states of above said SUSY partner pair. These tables (1, 2, 3, 4, 5, 6, 7, 8) clearly verify the mirror image property of these partner potentials. They have all the optimised and semi-classical energies identical. This is only possible when they are isospectral mirror image pair. Then from Fig. 3 it is completely clear that constructed SUSY partners are also mirror image to each other for a particular pair. The growth of these SUSY partner is same to the respective parent one (Fig. 2). Thus not only the energy but the mirror image property is also retained. These SUSY pairs are also isospectral mirror image pair. Thus, starting from one mirror image pair we have constructed another mirror image isospectral pair. The new pair is also SUSY partner of those potential. If one can apply SUSY theory again to construct the 2nd SUSY partner of the parent potentials, he will find another mirror image isospectral pair. Then, it is easy to conclude that starting from one mirror image pair and using SUSY theory one can construct infinite number of such pairs (if the parent potential is infinitely bound) whose energy spectrum is already known. These spectrums are known just by knowing the parent potential’s spectrum. Thus it

Table 6 Higher excited state energy calculation of the SUSY partner potentials of potential pair 2 to verify their mirror image property and Isospectrality using Wilson-Somerfield Quantisation Rule

n	\bar{E}_n of the parent isospectral pair	$\bar{E}_n(V_3^+)$	$\bar{E}_n(V_4^+)$
24		97.753 907 290 377 718 5100	97.753 907 290 377 718 5100
25	97.753 907 290 377 734 1		
49		197.750 450 515 161 378 349	197.750 450 515 161 378 349
50	197.750 450 515 161 421 65		
99		397.751 925 437 782 372 876	397.751 925 437 782 372 876
100	397.751 925 437 782 354 10		
199		797.752 473 696 908 635 05	797.752 473 696 908 635 05
200	797.752 473 696 908 245 34		
499		1997.775 562 782 265 521 46	1997.775 562 782 265 521 46
500	1997.775 562 782 265 678 12		
999		3997.753 984 218 464 870 9	3997.753 984 218 464 870 9
1000	3997.753 984 218 464 980 12		
1999		7997.766 461 830 199 487 8	7997.766 461 830 199 487 8
2000	7997.766 461 830 199 498 21		
4999		19997.767 416 489 838 450 4	19997.767 416 489 838 450 4
5000	19997.767 416 489 839 765 2		
9999		39997.767 085 284 751 880 5	39997.767 085 284 751 880 5
10000	39997.767 085 284 751 878 21		
49999		199997.790 443 169 135 156	199997.790 443 169 135 156
50000	199997.790 443 169 135 345 2		
99999		399997.808 699 337 234 690	399997.808 699 337 234 690
100000	399997.808 699 337 234 789 1		

not necessary that those isospectral potentials have to have common n th SUSY partner. Even, if they have SUSY partner isospectral to each other, then also one can construct isospectral partner potential. In this construction, mirror image property will play a major role.

At this end, one needs to concentrate on, the properties of this type of mirror image potential. Here for pair: 1 and pair: 3 the study has been done (Tables 9, 10). Ongoing calculation clearly indicates that they are obeying Eq. (10). Here for this variational calculation we choose $N = 50$. Thus with increase of state error in the optimised function increases as a result deviation between ΔT_n^2 and ΔV_n^2 increases. At this end one can easily conclude that these virial like properties are same for enantiomers. This means that all the physical properties related to hamiltonian are same for the enantiomers.

Thus one can say that in isospectral potential related by mirror image property have these essential properties same. Again one can say that analysing one partner of the pair he will get the essential information of the other pair. Thus, they have magnitude of $\langle x^l \rangle$ (l is odd) same but opposite in direction. As a matter of fact one can easily say that a pair of molecule having same molecular formula, and magnitude of

Table 7 Higher excited state energy calculation of the SUSY partner potentials of potential pair 3 to verify their mirror image property and Isospectrality using Wilson-Somerfield Quantisation Rule

n	\bar{E}_n of the parent isospectral pair	$\bar{E}_n(V_5^+)$	$\bar{E}_n(V_6^+)$
24		798.751 257 741 735 948 9	798.751 257 741 735 948 9
25	798.751 257 741 735 949 8		
49		2263.035 169 676 116 571 6	2263.035 169 676 116 571 6
50	2263.035 169 676 116 598 71		
99		6404.587 009 983 159 287 6	6404.587 009 983 159 287 6
100	6404.587 009 983 198 345 32		
199		18118.908 009 363 695 145	18118.908 009 363 695 145
200	18118.908 009 363 786 134		
499		71626.419 340 368 444 704	71626.419 340 368 444 704
500	71626.419 340 368 456 128		
999		202594.769 652 783 833 580	202594.769 652 783 833 580
1000	202594.769 652 783 841 25		
1999		573026.337 771 890 502 85	573026.337 771 890 502 85
2000	573026.337 771 890 543 24		
4999		2265091.804 266 307 831 3	2265091.804 266 307 831 3
5000	2265091.804 266 307 657 43		
9999		6406644.465 118 056 078	6406644.465 118 056 078
10000	6406644.465 118 056 078		
49999		71628666.381 092 427 807	71628666.381 092 427 807
50000	71628666.381 092 427 807		
99999		202595951.425 219 504 546	202595951.425 219 504 546
100000	202595951.425 219 513 564		

dipole moment can have identical spectrum. This conclusion can also be done if one considers individual bond moments. Because, it is expected that all the bond moment except one have same for both. And that particular moment is different in direction not in magnitude. Thus these types of potentials are a nice 1D model to enantiomeric potentials.

In this demonstration we try to get a compact form of the SUSY partner potential obeying the concept that, at $x \rightarrow \infty$ the parent and SUSY partner has the same behaviour. We have applied this scheme to potential pair: 1 and pair: 3 using polynomial curve fitting. The potential obtained in this scheme as follows.

For pair: 1

$$\bar{V}_1^+ = 2.1625925 + 0.7763113x + 1.7195307x^2 + 0.9436015x^3 + 0.9247491x^4$$

$$\bar{V}_2^+ = 2.1625925 - 0.7763113x + 1.7195307x^2 - 0.9436015x^3 + 0.9247491x^4$$

The correlation coefficient is 0.99999983 for both of the potential.

Range: ($-4 \leq x \leq 4$ and $0 \leq y \leq 1,000$)

Table 8 Higher excited state energy calculation of the SUSY partner potentials of potential pair 4 to verify their mirror image property and Isospectrality using Wilson-Sommerfeld Quantisation Rule

n	\bar{E}_n of the parent isospectral pair	$\bar{E}_n(V_7^+)$	$\bar{E}_n(V_8^+)$
24		1207.129 894 990 307 997 6	1207.129 894 990 307 997 6
25	1207.129 894 990 307 999 6		
49		3660.378 832 320 239 445 6	3660.378 832 320 239 445 6
50	3660.378 832 320 239 485 6		
99		11096.964 785 522 291 435 2560	11096.964 785 522 291 435 2560
100	11096.964 785 522 291 437 213		
199		33640.499 153 331 836 670	33640.499 153 331 836 670
200	33640.499 153 331 836 543		
499		145736.717 831 964 852 540	145736.717 831 964 852 540
500	145736.717 831 964 851 23		
999		441788.308 836 138 640 740	441788.308 836 138 640 740
1000	441788.308 836 138 6465 4		
1999		1339255.915 200 778 119 800	1339255.915 200 778 119 800
2000	1339255.915 200 778 134 12		
4999		5801848.995 977 019 956 3	5801848.995 977 019 956 3
5000	5801848.995 977 019 989 7		
9999		17588036.606 802 594 366 595 4	17588036.606 802 594 366 595 4
10000	17588036.606 802 594 387 34		
49999		230976498.870 380 444 434 170	230976498.870 380 444 434 170
50000	230976498.870 380 444 465 21		
99999		700189410.504 628 713 590	700189410.504 628 713 590
100000	700189410.504 628 713 618		

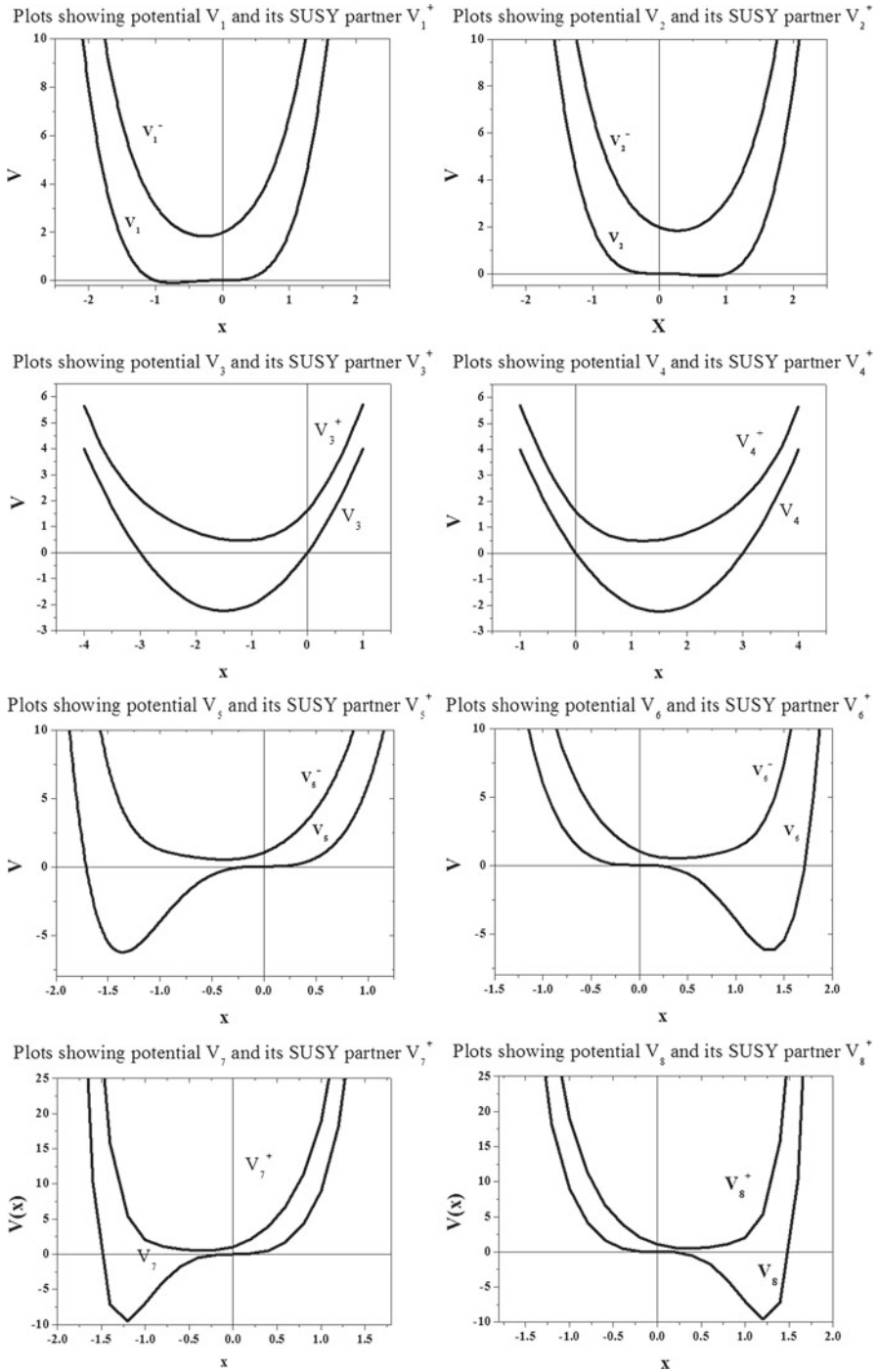


Fig. 2 Plot showing potential and its SUSY partner as a function of x

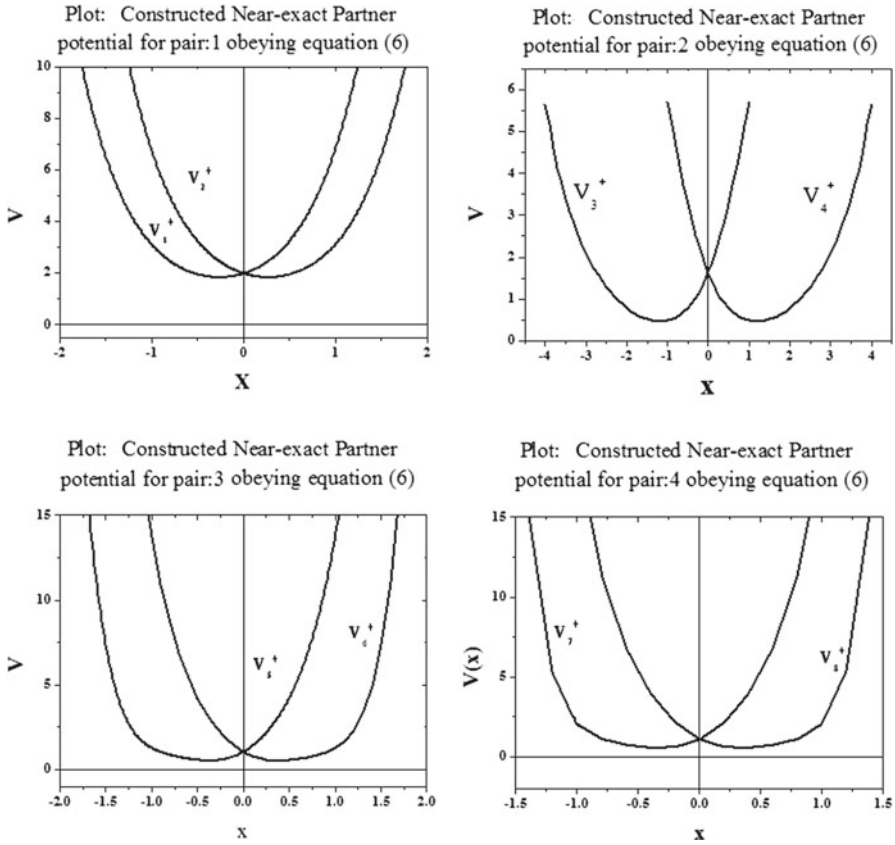


Fig. 3 Near-Exact SUSY partner potential for pair: 1–4 to show how these SUSY partner of respective pair related

For pair: 3

$$\begin{aligned} \bar{V}_5^+ &= 0.9412744 + 1.6341096x + 5.5752057x^2 + 4.5343999x^3 + 0.0529349x^4 \\ &\quad + 0.0264288x^5 + 0.9956145x^6 \\ \bar{V}_6^+ &= 0.9412744 - 1.6341096x + 5.5752057x^2 - 4.5343999x^3 + 0.0529349x^4 \\ &\quad - 0.0264288x^5 + 0.9956145x^6 \end{aligned}$$

The correlation coefficient is 0.99999978 for both of the potential.

Range: $(-3 \leq x \leq 3$ and $0 \leq y \leq 1,000)$

Here, initially the SUSY partner is constructed using optimised ground state wave function and obeying Eq. (8). Then using the point of that SUSY partner in a finite range these potentials are obtained so, error incurred in these potential is more. The solution is also same here. These potentials are diagonalised and the results are given in Table 11. Here the results are accurate upto 7–8 Again the interesting point is that these obtained potentials are also mirror image to each other. This also proves the effectiveness of

Table 9 ΔT_n^2 and ΔV_n^2 values for potential V_1 and V_2 obtain by using the variationally optimised wave function to show the validity of Eq. (10)

n	$(\Delta T_n^2(V_1))$	$(\Delta V_n^2(V_1))$	$(\Delta T_n^2(V_2))$	$(\Delta V_n^2(V_2))$
0	0.823 081 202 370 159 164	0.823 081 202 370 159 164	0.823 081 202 370 159 164	0.823 081 202 370 159 164
1	3.438 824 437 596 260 818	3.438 824 437 596 260 818	3.438 824 437 596 260 818	3.438 824 437 596 260 818
2	8.858 861 324 755 793 308	8.858 861 324 755 793 308	8.858 861 324 755 793 308	8.858 861 324 755 793 308
3	18.901 843 761 374 258	18.901 843 761 374 258	18.901 843 761 374 258	18.901 843 761 374 258
4	34.815 973 825 184 394	34.815 973 825 184 394	34.815 973 825 184 394	34.815 973 825 184 394
5	57.757 004 090 351 781	57.757 004 090 351 781	57.757 004 090 351 781	57.757 004 090 351 781
6	88.788 272 133 057 151	88.788 272 133 057 151	88.788 272 133 057 151	88.788 272 133 057 151
7	128.906 733 616 560 16	128.906 733 616 560 16	128.906 733 616 560 16	128.906 733 616 560 16
8	179.057 272 943 989 59	179.057 272 943 989 59	179.057 272 943 989 59	179.057 272 943 989 59
9	240.142 323 385 197 2	240.142 323 385 197 2	240.142 323 385 197 2	240.142 323 385 197 2
10	313.028 711 317 984	313.028 711 317 984	313.028 711 317 984	313.028 711 317 984
11	398.552 754 865 668	398.552 754 865 668	398.552 754 865 668	398.552 754 865 668
12	497.524 195 841 341	497.524 195 841 341	497.524 195 841 341	497.524 195 841 341
13	610.729 315 285 40	610.729 315 285 40	610.729 315 285 40	610.729 315 285 40
14	738.933 456 648 73	738.933 456 648 73	738.933 456 648 73	738.933 456 648 73
15	882.883 106 381 8	882.883 106 381 8	882.883 106 381 8	882.883 106 381 8
16	1043.307 635 693	1043.307 635 693	1043.307 635 693	1043.307 635 693
17	1220.920 777 55	1220.920 777 55	1220.920 777 55	1220.920 777 55
18	1416.421 893 1	1416.421 893 1	1416.421 893 1	1416.421 893 1
19	1630.497 068 6	1630.497 068 6	1630.497 068 6	1630.497 068 6

Table 10 ΔT_n^2 and ΔV_n^2 values for potential V_5 and V_6 obtain by using the variationally optimised wave function to show the validity of Eq. (7)

n	$(\Delta T_n^2(V_5))$	$(\Delta V_n^2(V_5))$	$(\Delta T_n^2(V_6))$	$(\Delta V_n^2(V_6))$
0	9.200 978 329 168 628 2	9.200 978 329 168 628 2	9.200 978 329 168 628 2	9.200 978 329 168 628 2
1	9.029 280 656 276 368	9.029 280 656 276 368	9.029 280 656 276 368	9.029 280 656 276 368
2	20.330 794 274 701 40	20.330 794 274 701 40	20.330 794 274 701 40	20.330 794 274 701 40
3	39.031 767 195 939 83	39.031 767 195 939 83	39.031 767 195 939 83	39.031 767 195 939 83
4	69.754 059 658 583 80	69.754 059 658 583 80	69.754 059 658 583 80	69.754 059 658 583 80
5	116.055 411 246 889 0	116.055 411 246 889 0	116.055 411 246 889 0	116.055 411 246 889 0
6	181.401 069 351 620	181.401 069 351 620	181.401 069 351 620	181.401 069 351 620
7	269.257 679 237 920	269.257 679 237 920	269.257 679 237 920	269.257 679 237 920
8	383.089 433 401 81	383.089 433 401 81	383.089 433 401 81	383.089 433 401 81
9	526.359 734 990 7	526.359 734 990 7	526.359 734 990 7	526.359 734 990 7
10	702.531 711 167 7	702.531 711 167 7	702.531 711 167 7	702.531 711 167 7
11	915.068 402 165 6	915.068 402 165 6	915.068 402 165 6	915.068 402 165 6
12	1167.432 830 131	1167.432 830 131	1167.432 830 131	1167.432 830 131
13	1463.088 024 15	1463.088 024 15	1463.088 024 15	1463.088 024 15
14	1805.497 028 48	1805.497 028 48	1805.497 028 48	1805.497 028 48
15	2198.122 904 11	2198.122 904 11	2198.122 904 11	2198.122 904 11
16	2644.428 728 0	2644.428 728 0	2644.428 728 0	2644.428 728 0
17	3147.877 590 8	3147.877 590 8	3147.877 590 8	3147.877 590 8
18	3711.932 595 1	3711.932 595 1	3711.932 595 1	3711.932 595 1
19	4340.056 855	4340.056 855	4340.056 855	4340.056 855

Table 11 Variational upper bound energies of the SUSY partner potentials (obtained by polynomial curve fitting) of mirror pair: 1 and 3

n	$\bar{E}_n(\bar{V}_1^+)$	$\bar{E}_n(\bar{V}_2^+)$	$\bar{E}_n(\bar{V}_5^+)$	$\bar{E}_n(\bar{V}_6^+)$
0	3.441 398 8	3.441 398 8	2.479 760 61	2.479 760 61
1	6.970 308 9	6.970 308 9	7.096 343 01	7.096 343 01
2	11.041 883 1	11.041 883 1	12.901 707 10	12.901 707 10
3	15.552 644 5	15.552 644 5	19.666 943 05	19.666 943 05
4	20.430 452 3	20.430 452 3	27.243 441 01	27.243 441 01
5	25.627 631 7	25.627 631 7	35.551 119 03	35.551 119 03
6	31.109 499 6	31.109 499 6	44.529 308 03	44.529 308 03
7	36.849 470 2	36.849 470 2	54.130 553 03	54.130 553 03
8	42.826 460 0	42.826 460 0	64.316 396 23	64.316 396 23
9	49.023 181 1	49.023 181 1	75.054 799 86	75.054 799 86
10	55.425 210 1	55.425 210 1	86.318 519 96	86.318 519 96
11	62.020 291 6	62.020 291 6	98.084 005 88	98.084 005 88
12	68.797 828 1	68.797 828 1	110.330 635 59	110.330 635 59
13	75.748 569 4	75.748 569 4	123.040 146 35	123.040 146 35
14	82.864 376 0	82.864 376 0	136.196 216 11	136.196 216 11
15	90.137 943 4	90.137 943 4	149.784 144 10	149.784 144 10
16	97.562 833 8	97.562 833 8	163.790 590 11	163.790 590 11
17	105.133 134	105.133 134	178.203 391 04	178.203 391 04
18	112.843 4334	112.843 434	193.011 370 22	193.011 370 22

mirror image property. Thus mirror image pairs have mirror image SUSY partners. Finally a recipe is given to construct infinite number of pair of isospectral potential starting from one pair. Again a compact form of the SUSY pair is obtained for this type of potentials. This fitting concept concretely proves the mirror image nature of the SUSY partners and can be applied to any potential during construction of their SUSY partner in a compact form. Mirror image potentials are very good 1D model to enantiomers. From this discussion one can say that SUSY partners of the enantiomers are nothing but other enantiomers. SUSY theory involving mirror image potentials can easily be used now, in constructing a series of enantiomers.

6 Conclusions

In summary, we have put forward here a scheme of testing the Isospectrality in a rigorous manner, only by using mirror image property of a pair of potential. To this end, we first obtain a pair of exact isospectral partner potential for problems that are not exactly solvable. We have successfully derived the 1D model to enantiomers. Then also we have found to offer sufficiently precise SUSY partner Hamiltonians H^+ for all the cases under consideration. This is verified by spectral studies for quite a few energy levels of H^+ and by analyzing the nature of V versus V^+ plots. The observations are specifically noteworthy because the latter entails a first order error. Our error analysis

is particularly relevant to studies involving a hierarchy of SUSY Hamiltonians that are constructed with a view to allowing one to employ a smaller basis set for calculations of excited-state energies. We have also indicated a way of simplifying the forms of the partner potentials. The, obtained SUSY pair are also mirror image to each other. Thus one can expect the 2nd SUSY partners are also mirror image pair and so on. Thus a new family of SUSY pair is been created where each SUSY partner is mirror image to the corresponding other member of the pair. This should be quite rewarding in view of the close kinship of the SUSY theory with isospectral molecules and nanostructures and their thermodynamical features.

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