SUSY QM in a One-Dimensional Box and Local Observable Quantities

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We investigate several Hamiltonians for a free particle in a one-dimensional box, in the context of supersymmetric quantum mechanics. Specifically, we study this problem with the Neumann boundary condition, the periodic and antiperiodic boundary condition, and some mixed and complex boundary conditions. This is achieved by using an approach recently proposed which expresses the factorization of the partner Hamiltonians in terms of the probability density and current for the ground-state eigenfunction of one of them.

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As is well known, one of the methods used in quantum mechanics for finding new exactly solvable potentials with almost equal energy spectra is the so-called factorization method (this powerful tool of quantum mechanics goes back to Schrödinger’s works,[1] although the technique appeared first in Dirac’s renowned book[2]). Its modern version is also known as the intertwining technique between a pair of partner operators (Hamiltonians). After Witten’s celebrated work,[3] it was noted that the supersymmetric quantum mechanics (SUSY QM) as nowadays called was essentially equivalent to the factorization method.[4] In the last years, SUSY QM has become a very active field of research as is particularly shown in Refs.[5,6].

For example, extensive studies that involve exactly solvable potentials have been carried out. Until a short time ago, the supersymmetric version of the simplest model problem of quantum mechanics with bound states—the free particle inside a one-dimensional box (with Hilbert space \( L^2(\Omega) \), where \( \Omega \subset \mathbb{R} \))—had been studied only when the ground state eigenfunction for the Hamiltonian \( \hat{H} \) satisfies the Dirichlet boundary condition.[7] Recently, another boundary condition (nonstandard) was considered for this same problem,[8] also introducing an alternative approach to the general problem of factorization that uses the probability density and current corresponding to the ground-state eigenfunction of \( \hat{H} \) (for a particle in a box this eigenfunction could be complex). The SUSY quantum mechanical treatment of the infinite square well potential (with Hilbert space \( L^2(\mathbb{R}) \)) has also been studied.[9] There, the SUSY version of the finite square well potential was developed first, and then from these results, the corresponding infinite square well was obtained.

In this Letter we complement the procedure introduced in Ref.[8] and illustrate it by supersymmetricizing several specific examples of Hamiltonians that describe a free particle inside a one-dimensional box. All the energy eigenvalues of these Hamiltonians are fully discrete and we focus on them here. As far as we know, this simple problem (with others solvable with explicit boundary conditions) has not been considered in the literature until now. We believe that our approach, with local observable quantities, is specially useful for consideration of bound states, moreover it complements the general SUSY complexification procedure studied by Andrianov et al.[10] and Bagchi et al.,[11] but in our case, one of the partner potentials is real and the other is complex (this specific situation has also been considered in Ref.[12] and more recently in Ref.[13]).

Let us assume that the real Hamiltonian \( \hat{H} \) has eigenvalues \( E_n \) and eigenfunctions \( \psi_n(x) \) which are explicitly known. Here \( n = 0, 1, 2, \ldots \) is ordered by increasing energy. The ground-state eigenfunction is \( \psi_0(x) \) and its corresponding energy is \( E_0 \) (we took \( E_0 = 0 \) in Ref.[8]). We write

\[
\hat{H}\psi_0(x) = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi_0(x) = E_0\psi_0(x),
\]

We first express \( \psi_0(x) \) in polar form \( \psi_0(x) = R_0(x) \exp \left( \frac{i S_0}{\hbar} \right) \), and then substitute it in Eq. (1). Upon separation into real and imaginary parts, Eq. (1) yields a pair of equations:

\[
-\frac{\hbar^2}{2m} R'_0 - \frac{1}{\hbar^2} R_0 (S'_0)^2 + V(x) R_0 = E_0 R_0,
\]

\[
-\frac{\hbar^2}{2m} \frac{2}{\hbar} R'_0 S'_0 + \frac{1}{\hbar} R_0 S'_0 = 0,
\]

where \( R_0(x) = |\psi_0|^2 \) is the probability density for \( \psi_0(x) \) (in principle, \( R_0(x) \) has no zeros because this is a specific feature of the ground state). Its corresponding probability current \( j_0(x) = \frac{\hbar}{m} \text{Im}(\psi_0^* \psi_0') \) gives

\[
\frac{1}{m} R_0^2 S'_0. \text{ Thus, we can write Eq. (3) as } -\frac{\hbar^2}{2m} j'_0 = 0 \quad (\Rightarrow j_0 = \text{const}), \text{ which is satisfied if } V(x) \text{ is a real}
\]

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potential and therefore \( \hat{H} \) can be self-adjoint. Then from Eq. (2) we obtain
\[
V(x) = \frac{\hbar^2}{2m} \frac{R_0''(x)}{R_0(x)} - \frac{m}{2} \frac{j_0^2}{R_0^2(x)} + E_0.
\]
(4)

This expression also takes the suggestive form
\[
\frac{m}{2}(v_0)^2 + V(x) + Q_0(x) = E_0,
\]
where \( v_0(x) = \frac{j_0}{R_0(x)} \), and
\[
Q_0(x) = \frac{\hbar^2}{2m} \frac{R_0''(x)}{R_0(x)}
\]
are the Bohmian velocity and the Bohm quantum potential (corresponding to the ground-state eigenfunction), respectively.

With the potential \( V(x) \), the Hamiltonian \( \hat{H} \) introduced in Eq. (1) is subsequently given by
\[
\hat{H} = \hat{b} \hat{a} + E_0,
\]
(5)

where the following linear differential operators are defined
\[
\hat{a} = \frac{\hbar}{\sqrt{2m}} \left( \frac{d}{dx} - \frac{R_0'(x)}{R_0(x)} \right),
\]
\[
\hat{b} = \frac{\hbar}{\sqrt{2m}} \left( -\frac{d}{dx} - \frac{R_0'(x)}{R_0(x)} \right) - \frac{ij_0}{\hbar} \frac{1}{R_0^2(x)}.
\]
(6)

If the typical case \( j_0 = 0 \) is considered, in which case \( \psi_0^* \psi_0 \) is real (for example, choosing the ground-state eigenfunction \( \psi_0 \) to be real), one has (formally) \( \hat{b}^* = \hat{a} \). It is important to note that \( \hat{b} \psi_0(x) = 0 \), but automatically \( \hat{a} \psi_0(x) = 0 \) (even if \( j_0 \neq 0 \)). That is, \( \psi_0(x) \), which is normalizable, is annihilated by the operator \( \hat{a} \).

A new SUSY partner Hamiltonian \( \hat{H}_S = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_S \) (with eigenvalues and eigenfunctions denoted by \( E_S \) and \( \psi_S \), respectively) may be constructed: that is,
\[
\hat{H}_S = \hat{a} \hat{b} + E_0,
\]
(7)

where the complex potential \( V_S(x) \) is
\[
V_S(x) = -\frac{\hbar^2}{2m} \frac{R_0''(x)}{R_0(x)} + \frac{\hbar^2}{m} \frac{(R_0')^2(x)}{R_0^2(x)} - \frac{m}{2} \frac{j_0^2}{R_0^2(x)} + i2\hbar j_0 \frac{R_0'(x)}{R_0^2(x)} + E_0.
\]
(8)

From Eqs. (5) and (7) it is clear that there is an intertwining between the operators \( \hat{H} \) and \( \hat{H}_S \):
\[
\hat{H}_S \hat{a} = \hat{a} \hat{H},
\]
(9)
\[
\hat{b} \hat{H}_S = \hat{H} \hat{b}.
\]
(10)

The latter relation is equal to
\[
(\hat{a}^*)^+ \hat{H}_S = \hat{H}(\hat{a}^*)^+,
\]
(11)
and is obtained from Eq. (9) taking its complex conjugation, and then its formal adjoint (it must be recalled that \( \hat{H} \) is real but, in general, \( \hat{H}_S = (\hat{H}_S)^+ \) is complex). Remarkably, if \( \psi(x) \) is a solution of the Schrödinger eigenvalue equation \( \hat{H} \psi = E \psi \), then \( \psi_S(x) \sim (\hat{a} \psi)(x) \neq 0 \) is a solution of the equation \( \hat{H}_S \psi_S = E \psi_S \) with the same energy \( E \). The solutions \( \psi \) and \( \psi_S \) can only be considered eigenfunctions of \( \hat{H} \) and \( \hat{H}_S \), respectively, if they are physically adequate, i.e. if they satisfy proper boundary conditions and are normalizable.

The potentials \( V(x) \) and \( V_S(x) \) may also be written as
\[
V(x) = w^2(x) - \frac{\hbar}{\sqrt{2m}} w'(x) + E_0,
\]
(12)
\[
V_S(x) = w^2(x) + \frac{\hbar}{\sqrt{2m}} w'(x) + E_0,
\]
where the complex quantity
\[
w(x) = \frac{\hbar}{\sqrt{2m}} \left( -\frac{R_0'(x)}{R_0(x)} - \frac{1}{\hbar} \frac{ij_0}{R_0^2(x)} \right),
\]
(13)
is the so-called superpotential. Note that \( w(x) = \frac{h}{\sqrt{2m}} \psi_0(x) \) satisfies the well-known Ricatti equation (usually \( V(x) \) or \( V_S(x) \) is given).

In order to take contact with a general SUSY complexification procedure studied in Ref. [11], let us write \( w(x) \equiv W(x) = f(x) + ig(x) \) (Eq. (2.12) in Ref. [11]) with \( h = 2m \equiv 1 \), so from Eq. (13) we have
\[
f(x) = -\frac{R_0'(x)}{R_0(x)}, \quad g(x) = -\frac{j_0}{2} \frac{1}{R_0^2(x)}.
\]
Substituting these expressions in our Eq. (4) and Eq. (8) we obtain relations (2.20)–(2.23) in Ref. [11],
\[
V_R^{(+)} = \text{Re}(V(x)) = f^2(x) - g^2(x) - f'(x) + E_0,
\]
\[
V_L^{(+)} = \text{Im}(V(x)) = 0,
\]
\[
V_R^{(-)} = \text{Re}(V_S(x)) = f^2(x) - g^2(x) + f'(x) + E_0,
\]
\[
V_L^{(-)} = \text{Im}(V_S(x)) = 2f(x)g(x) + g'(x),
\]
with \( E_0 \equiv E_R \) and \( E_I = 0 \) (see Ref. [11]).

In order to demonstrate the usefulness of our approach, we choose several Hamiltonians \( \hat{H} \) that describe a free particle in a box with walls at \( x = 0 \) and \( x = L \). It is known that there exists a four parameter family of self-adjoint Hamiltonians (boundary conditions) for this system. For some of these boundary conditions, it can be demonstrated that the corresponding ground-state eigenfunction verifies \( j_0 = 0 \); suggesting in general, impenetrability at the walls of the box. If one has that \( j_0 \neq 0 \), this physically corresponds to a particle in the box but not confined at all to the box. Thus, from the infinite set
of boundary conditions included within the four parameter family, we will study the following: (a) Neumann condition: \( \psi'(0) = \psi'(L) = 0 \), (b) a mixed condition:
\[
\psi(0) = \psi(L) = 0,
\]
(c) another mixed condition:
\[
\psi'(0) = \psi(L) = 0,
\]
(d) periodic condition: \( \psi(0) = \psi(L) \), \( \psi'(0) = \psi'(L) \), (e) antiperiodic condition:
\[
\psi(0) = -\psi(L), \quad \psi'(0) = -\psi'(L),
\]
(f) a complex condition: \( \psi(0) = i\psi(L), \quad \psi'(0) = i\psi'(L) \), (g) another complex condition:
\[
\psi(0) = -i\psi(L), \quad \psi'(0) = -i\psi'(L).
\]

Let us begin by summarizing the programme that we will follow. Firstly, one obtains the eigenfunctions \( \psi_n(x) \) of the Hamiltonian \( \hat{H} \) with eigenvalues \( E_n \) (the ground-state energy is adjusted so that \( E_0 = 0 \), so that \( V(x) \) is not always zero). The observable quantities \( R_0(x) \) and \( j_0 \) are obtained from \( \psi_0(x) \). Using Eq. (13) it is now easy to find the superpotential \( w(x) \). From here on, we can obtain the corresponding supersymmetric partner potential \( V_S(x) \) for a particle in a box in the potential \( V(x) \) (using Eq. (12)). The eigenfunctions of \( V_S(x) \) are obtained from \( \psi_S(x) \sim (\hat{a}^\dagger)(x) \), where the operator \( \hat{a} \) is calculated in Eq. (6). The Hamiltonians \( \hat{H} \) and \( \hat{H}_S \) have the same energy levels except for the ground state. From now on we write \( h^2 = 2m = 1 \) and the box width has been chosen to be \( L = \pi \). The quantities \( R_0 \) and \( j_0 \) are always written for \( \psi_0 \) normalized and \( n \) is a positive integer \( (n \geq 0) \) except where otherwise indicated. Thus, the following results are obtained: (a) We have \( V(x) = 0, \ E_n = n^2 \) and \( \psi_n(x) \sim \cos(nx) \), then \( j_0 = 0 \) and also \( R_0(x) = \sqrt{n/\pi} \). The superpotential is null \( w(x) = 0 \). From these results we obtain \( V_S(x) = 0 \) and \( (E_S)_n = (n + 1)^2 \). The eigenfunctions of \( V_S(x) \) are \( (\psi_S)_n \sim \sin((n + 1)x) \) which are precisely those corresponding to the free particle inside a box with Dirichlet boundary condition. That is, the standard supersymmetric partner potential \( V_S(x) \) of \( V(x) = 0 \) with Neumann boundary condition is the potential for the infinite square well. This is indeed a very nice result. Note that a situation also interesting is met if one starts (inadvertently) from the first excited eigenfunction \( \psi_1(x) \), that is, from its corresponding probability density \( R_1(x) = \sqrt{2/\pi} \cos(x) \) and probability current \( j_1 = 0 \), which implies \( w(x) = \tan(x) \). For these choices the partner potentials and corresponding eigenvalues are \( V(x) = -1 \) and \( E_n = n^2 - 1 \), so that \( E_0 = -1 \) and \( E_1 = 0 \). Likewise, we obtain the potential \( V_S(x) = 2\sec^2(x) - 1 \) with spectra \( (E_S)_n = 4(n + 1)(n + 2) \) and eigenfunctions \( (\psi_S)_n \sim (2n + 3)\sin(2n + 3)x - \tan(x)\cos(2n + 3)x \). In this last factorization \( V_S(x) \) (and the superpotential) is singular at \( x = \pi/2 \), which requires the wave function to vanish there. Thus, the almost absolute equality for the spectra of \( V(x) \) and \( V_S(x) \) is not valid. (b) We have in this case \( V(x) = -1/4 \), \( E_n = n(n + 1) \) and \( \psi_n(x) \sim \sin((2n + 1)x/2) \). Then \( j_0 = 0 \) and \( R_0(x) = \sqrt{2/\pi}\sin(x/2) \). The superpoten-
functions \((\psi_{S})_{n}\) which can be obtained from \(\psi_{n}(x)\) making the change \(n \rightarrow n + 1\). This complex set of functions is obviously not complete. (g) We have in this case similar results to \(V(x), E_{n}, j_0\) and \(R_{0}(x)\) as in the latter case, but \(\psi_{n}(x) \sim \exp(i(-1)^{n}(2n + 1)x/2)\), which implies \(w(x) = -i/2\). We obtain \(V_{S}(x) = -1/4\) and \((E_{S})_{n} = (n + 1)(n + 2)\) as in boundary condition (f). The complex set of functions \((\psi_{S})_{n}\), obtained from \(\psi_{n}(x)\) making the change \(n \rightarrow n + 1\), is not complete again.

In conclusion, we have complemented and illustrated the approach introduced in Ref.[8] by supersymmetrizing several specific examples of Hamiltonians that describe a free particle inside a one dimensional box. We have found some interesting results: the standard supersymmetric partner Hamiltonian \((\hat{H}_{S})\) of \(\hat{H}\) with \(V(x) = 0\) and Neumann boundary condition is precisely the Hamiltonian for the standard infinite square well. It must be noted that when we apply a boundary condition like \(\psi(0) = 0\) or \(\psi(L) = 0\), the same condition is fulfilled by the function \(\psi_{S}\) and its derivative. Likewise, when we impose \(\psi' = 0\) at one wall, the function \(\psi_{S}\) is zero there. On the other hand, the set of functions \((\psi_{S})_{n}\) for an operator \(\hat{H}_{S}\) may not be complete when we have complex eigenfunctions for \(\hat{H}\) and also real eigenfunctions (with ground state non degenerate), in this case, we have to add to this set the function \(\psi_{0}\); nevertheless, \(E_{S} = 0\) does not belong to the spectral set of \(\hat{H}_{S}\). Finally, owing to the chosen boundary conditions, the study in this Letter has been limited to real potential partners \(V_{S}(x)\). However, we may also obtain complex valued potentials \(V_{S}(x)\) with real spectra if \(j_{0} \neq 0\) and \(R_{0} \neq 0\); in all these cases \(\psi_{0}\) must be a non trivial complex solution (i.e. different to \(\exp(\pm iCx)\)) of the eigenvalue equation \(\hat{H}_{S}(x) = E_{0}\psi_{0}(x)\) with \(V(x) = \text{const}\) (which may have an analytical solution, i.e. solvable explicitly). Working on this topic is in progress.

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References

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