Alternative approach to the Schrödinger equation: Shifting operators between Hilbert spaces

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For a given one-dimensional Hamiltonian we construct a family of Hamiltonians whose Hilbert spaces are related by shifting operators such that each level of the original Hilbert space corresponds to the ground state of another one of the family. This allows us to establish the equivalence between the Schrödinger equation and a sequence of Ricatti equations.

I. INTRODUCTION

Recently Mielnik presented a paper¹ with an interesting derivation based on the factorization method for a family of potentials with the same spectrum as that of the harmonic oscillator. On the other hand, P. Kumar et al ² uses a supersymmetric partner of the anharmonic-oscillator Hamiltonian in order to evaluate approximately the first excited state of the latter using the ground state of the former. These works can be embedded in a wider perspective so as to obtain an alternative technique to solve the eigenvalue problem as it appears in quantum mechanics. This is the aim of the present work. Unlike the classical method which consists in finding general solutions for the Schrödinger equation and then determining the energy values consistent with the boundary conditions, this method allows us to obtain in a sequential way the eigenvalues and eigenfunctions for a given potential from the ground state. In this aspect it reminds us of the method based on the usual ladder operators, $3,4$ but here we use shifting operators between Hilbert spaces, and generate as a primary ingredient a sequence of ground states whose eigenvalues integrate the searched spectrum.

To set forth this approach we build from a given Hamiltonian $H^{(0)}$ a sequence of Hamiltonians $\{H^{(n)}\},\$ such that given a pair of consecutive Hamiltonians of the sequence, their spectra are the same except for a truncation of the ground state. That way the eigenvalue for the first excited state of $H^{(n)}$ coincides with that corresponding to the ground state of $H^{(n+1)}$, and so on. In general, given

$$
H^{(n)}\psi_m^{(n)} = \epsilon_m^{(n)} \t\t(1)
$$

we will have

$$
\epsilon_m^{(n)} = \epsilon_{m-1}^{(n+1)}, \quad m \ge 1 \tag{2}
$$

We get this by using operators that connect the Hilbert spaces $\mathcal{H}^{(n)}$ of the Hamiltonians $H^{(n)}$ among them. They are obtained by an adequate factorization of the $H^{(n)}$'s. At this point we make contact with the factorization method of Infeld and Hull.³

Using this structure, the determination of the spectrum of a given Hamiltonian $H^{(0)}$ is reduced to the evaluation of a sequence of ground states. The latter has an interesting advantage, as the calculation of such states is particularly simple, either in exact form or in a perturbative one, compared with that of excited states. The Hilbert space of the system, $\mathcal{H}^{(0)}$, is given by the application of the shifting operators between Hilbert spaces, $A^{(n)}$ and $A^{(n)^{\dagger}}$.

$$
\psi_m^{(n)} \sim A^{(n)^{\dagger}} \psi_{m-1}^{(n+1)} \; ; \tag{3}
$$

therefore

$$
\psi_m^{(0)} \sim A^{(0)^{\dagger}} A^{(1)^{\dagger}} \cdots A^{(m-1)^{\dagger}} \psi_0^{(m)} . \tag{4}
$$

On the other hand, the formulation of the Schrodinger equation in terms of the Ricatti equation has awakened nterest for years, particularly in relation with the perturbation theory.^{5,6} For one-dimensional problems it gives place to a scheme where the perturbative solutions can be obtained in quadrature for any order in terms of the nonperturbed solutions and the perturbative potential. But this method has the drawback that its application is dificult if the wave function has nodes, and for this reason it has been used mainly for first-order approximations for excited states. However, it is of simple and direct application in the case of a ground state, both in the exact and the perturbative evaluation.

In this work we combine both ingredients: the use of the shifting operators between Hilbert spaces, in order to reduce the determination of the spectrum and the eigenfunctions of a given Hamiltonian to a sequence of ground states, and the application of the Ricatti equation to evaluate these ground states.

The work is organized as follows. In Sec. II we give a brief review of the use of the Ricatti equation in the case of a ground state. In Sec. III we show the factorization of the Hamiltonian and the construction of a partner Hamiltonian, which has the same Hilbert space except for the truncated ground state. In Sec. IV we restate the Schrödinger problem as a sequence of Ricatti equations, developing the mentioned family of Hamiltonians $\{H^{(n)}\}$. Section V contains two simple example, and finally in Sec. VI we make some general comments.

II. THE GROUND STATE AND THE RICATTI EQUATION

The wave function for the ground state has no nodes; therefore, we can write it as

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$$
\psi_0 \sim \exp\left(\int_0^x dy \, g\left(y\right)\right) \,,\tag{5}
$$

where $g(y)$ is a regular function, without poles. Replacing it in the Schrödinger equation,

$$
H\psi_0 \equiv \left(-\frac{1}{2}\frac{d^2}{dx^2} + V(x)\right)\psi_0(x) = \epsilon_0\psi_0(x) , \qquad (6)
$$

we obtain the well-known Ricatti equation

$$
\frac{1}{2}(g^2+g') - V + \epsilon_0 = 0 \tag{7}
$$

The solution of this equation gives us directly the ground state, which has been isolated from the Hilbert space by the transformation (5). Although it cannot be solved for an arbitrary potential in a closed form, for a great number of usual systems in quantum mechanics $g(x)$ and ϵ_0 can be determined without difficulty.

Furthermore, in these terms we can easily obtain the first-order differential operator that annihilates the ground state. Defining it by

$$
A\,\psi_0=0\tag{8}
$$

and taking into account Eq. (5), we have

$$
A \sim \frac{d}{dx} - g(x) \tag{9}
$$

Let us remark that this operator that corresponds, as we will see further on, to a factorization of the Hamiltonian, has in general no connection with ladder operators in the Hilbert space because it does not relate its different states.

III. THE FACTORIZATION OF THE SCHRÖDINGER OPERATOR

From here on, in a rather obvious notation, we will use a superscript to indicate the different Hamiltonians and related quantities From $A^{(0)}$ we can build the following second-order Hermitian operators:

$$
A^{(0)^{\dagger}} A^{(0)} = -\frac{d^2}{dx^2} + (g^{(0)^2} + g^{(0)'}) , \qquad (10)
$$

$$
A^{(0)}A^{(0)^{\dagger}} = -\frac{d^2}{dx^2} + (g^{(0)^2} - g^{(0)}) , \qquad (11)
$$

where $g^{(0)} = (d/dx)g^{(0)}$. The interpretation of the first operator is straightforward. From (6) and (7), it corresponds to $2H^{(0)}$ with a shift in the energy such that the ground-state energy is zero:

$$
\tilde{H}^{(0)} \equiv \frac{1}{2} A^{(0)^{\dagger}} A^{(0)} = H^{(0)} - \epsilon^{(0)} . \tag{12}
$$

We now have to evaluate the meaning of (11). $\tilde{H}^{(0)}$ is an Hermitian operator; therefore, its eigenvalues are positive definite except the one of the ground state, which is zero:

$$
A^{(0)^{\dagger}} A^{(0)} u = \lambda^2 u \tag{13}
$$

For $\lambda \neq 0$ we can define

$$
A^{(0)}u = \lambda v \tag{14}
$$

(5) from which follows

$$
A^{(0)}v = \lambda u \tag{15}
$$

but this implies

$$
A^{(0)} A^{(0)} v = \lambda^2 v \tag{16}
$$

This shows that $\frac{1}{2}A^{(0)}A^{(0)^{\dagger}} \equiv H^{(1)}$ is an Hermitian operator with the same spectrum as $\tilde{H}^{(0)}$, except for the eigenvalue corresponding to its ground state. The ground-state energy of $H^{(1)}$ is the energy of the first excited state of $\widetilde{H}^{(0)}$:

$$
\epsilon_0^{(1)} = \tilde{\epsilon}_1^{(0)} = \epsilon_1^{(0)} - \epsilon_0^{(0)} \tag{17}
$$

or

$$
\epsilon_1^{(0)} = \epsilon_0^{(1)} + \epsilon_0^{(0)} \tag{18}
$$

The structure of this pair of correlated Hamiltonians can be considered as a manifestation of a supersymmetry underlying the Schrödinger equation.^{2,7}

IV. THE SHIFTING OPERATORS BETWEEN HILBERT SPACES AND THE RICATTI SEOUENCE

With the elements given in Secs. II and III we can now develop the approach outlined in Sec. I. Redefining the operator $H^{(1)} = \frac{1}{2} A^{(0)} A^{(0)^T}$, by a shifting $\epsilon_0^{(1)}$ in the energy, we have

$$
\widetilde{H}^{(1)} = H^{(1)} - \epsilon_0^{(1)} = -\frac{1}{2} \frac{d^2}{dx^2} + \widetilde{V}^{(1)}
$$
\n(19)

with

$$
\widetilde{V}^{(1)} = \frac{1}{2} (g^{(0)^2} - g^{(0)'}) - \epsilon_0^{(1)} \ . \tag{20}
$$

The ground state of $\tilde{H}^{(1)}$ has zero energy, and will satisfy the Ricatti equation

$$
\frac{1}{2}(g^{(1)^2}+g^{(1)'})-\frac{1}{2}(g^{(0)^2}-g^{(0)'})+\epsilon_0^{(1)}=0,
$$
\n(21)

and finally, by using Eq. (7), we obtain

$$
g^{(1)^2} + g^{(1)'} = 2V - 2(g^{(0)'} + \epsilon_0^{(0)}) - 2\epsilon_0^{(1)}.
$$
 (22)

This equation gives us both $g^{(1)}$ and $\epsilon_0^{(1)}$.

Of course, it is possible to iterate the previous transformation and get a new Hamiltonian,

$$
H^{(2)} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} (g^{(1)^2} - g^{(1)}) \tag{23}
$$

whose ground state corresponds to the first excited state of $H^{(1)}$, and to the second one of $H^{(0)}$. This process can be continued until we find a Ricatti equation without a solution, which points to the existence of an upper bound for the spectrum.

Resuming, the sequence of Ricatti equations thus generated is equivalent to the Schrödinger equation (6), and has the following generic expression:

$$
\frac{1}{2}(g^{(n)^2}+g^{(n)'})=V(x)-\sum_{m=0}^{n-1}(g^{(m)'}+\epsilon_0^{(m)})-\epsilon_0^{(n)},
$$

$$
n=0,1,2,\ldots, (24)
$$

as can be straightforwardly proved by complete induction.

The eigenvalue for the *n*th state of $\vec{H}^{(0)}$ is, iterating (18),

$$
\epsilon_n^{(0)} = \sum_{m=0}^n \epsilon_0^{(m)} \,, \tag{25}
$$

and the corresponding eigenfunction, from Eq. (15), is given by

$$
\psi_n^{(0)} = A^{(0)^{\dagger}} A^{(1)^{\dagger}} \cdots A^{(n-1)^{\dagger}} \psi_0^{(n)}, \qquad (26)
$$
 and

with

$$
A^{(m)} = \frac{d}{dx} - g^{(m)}(x) \tag{27}
$$

the shifting operators between Hilbert spaces.

V. EXAMPLES

In this section we present two simple examples, in order to show how this method works.

A. The harmonic oscillator

This is a rather peculiar system, in the sense that it has an equally spaced spectrum. This will be reflected in the very simple structure of the Ricatti sequence. We have

$$
V(x) = \frac{1}{2}x^2\tag{28}
$$

and Eq. (24) for $n = 0$ gives

$$
g^{(0)^2} + g^{(0)'} = x^2 - 2\epsilon_0^{(0)}.
$$
 (29)

The general solution for this equation is

$$
g^{(0)} = -x + \beta \frac{e^{x^2}}{1 + \beta \int_0^x dy \, e^{y^2}} \tag{30}
$$

with

$$
\epsilon_0^{(0)} = \frac{1}{2} \tag{31} \epsilon_0^{(0)} = \frac{1}{2}
$$

$$
\psi_0^{(0)} \cong \left[1 + \beta \int_0^x dy \, e^{y^2}\right] e^{x^2/2} \,, \tag{32}
$$

but only the normalizable solutions are the relevant ones. This implies $\beta = 0$, and, therefore,

$$
g^{(0)} = -x \tag{33}
$$

and

 $\psi_0^{(0)} \sim e^{-x^2/2}$

For
$$
n = 1
$$
 we have

$$
g^{(1)^{2}} + g^{(1)'} = 2V - 2(g^{(0)'} + \epsilon_{0}^{(0)}) - 2\epsilon_{0}^{(1)}
$$

= $x^{2} + 1 - 2\epsilon_{0}^{(1)}$, (34)

and the solution is

$$
g^{(1)} = -x, \quad \epsilon_0^{(1)} = 1 \tag{35}
$$

and from here on

$$
g^{(n)^2} + g^{(n)'} = x^2 + 1 - 2\epsilon_0^{(n)},
$$
\n(36)

which implies

$$
g^{(n)} = -x, \quad \epsilon_0^{(n)} = 1 \tag{37}
$$

Taking this into account we finally have

$$
\epsilon_n^{(0)} = \epsilon_0^{(0)} + \sum_{m=1}^n \epsilon_0^{(m)} = \frac{1}{2} + n \tag{38}
$$

$$
\psi_n^{(0)}(x) \sim \left(\frac{d}{dx} - x\right)^n e^{-x^2/2},
$$
\n(39)

the well-known solution for the harmonic oscillator.

B. A central potential

The radial Schrödinger equation for potential $V(r) = \alpha/r$ is

$$
\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \left[\frac{l(l+1)}{r^2} - \frac{\alpha}{r}\right]\bigg|\psi = \epsilon\psi\tag{40}
$$

and defining $\psi=(1/r)\chi$, the problem is reduced to the Hamiltonian

$$
H^{(0)} = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{1}{2} \left[\frac{l(l+1)}{r^2} - \frac{\alpha}{r} \right],
$$
 (41)

with $\epsilon^{(0)} = -(1/2)\epsilon$. For $n = 0$, Eq. (24) is now

> $^{(0)}^{2} + g^{(0)} = \frac{l(l + 1)}{r^{2}} - \frac{\alpha}{r} - 2\epsilon_0^{(0)}$ (42)

and the solution is given by

$$
g^{(0)} = \frac{l+1}{r} - \frac{\alpha}{2(l+1)},
$$

$$
\epsilon_0^{(0)} = \frac{\alpha^2}{8(l+1)^2};
$$
 (43)

and thus therefore, the wave function is, from Eqs. (26) and (27),

32)
$$
\chi_0^{(0)} \sim r^{1+1} e^{-\left[\alpha/2\left(l+1\right)^r\right]} \ . \tag{44}
$$

For $n = 1$, we have

$$
g^{(1)^2} + g^{(1)'} = \frac{(l+1)(l+2)}{r^2} - \frac{\alpha}{r} + \frac{\alpha^2}{4(l+1)^2} - 2\epsilon_0^{(1)}, \quad (45)
$$

which gives

$$
g^{(1)} = \frac{l+2}{r} - \frac{\alpha}{2(l+2)},
$$

\n
$$
\epsilon_0^{(1)} = \frac{\alpha^2}{8(l+1)^2} \frac{1+2(l+1)}{(l+2)^2}.
$$
\n(46)

From Eqs. (25) , (43) , and (46) , we have

$$
\epsilon_1^{(0)} = \epsilon_0^{(0)} + \epsilon_0^{(1)} = \frac{\alpha^2}{8(l+2)^2}
$$
 (47) $\left(-\frac{1}{2}\frac{d}{dx}\right)$

and so on. Of course, it is easy to find the solution for an arbitrary level, as in the preceding example. The corresponding expressions are

$$
g^{(n)} = \frac{a^{(n)}}{r} + b^{(n)} \t{,} \t(48)
$$

with

$$
a^{(n)}=l+1+n
$$
, $b^{(n)}=-\frac{\alpha}{2(l+1+n)}$

and

$$
\epsilon_0^{(n)} = -\frac{\alpha^2}{8} \left[\frac{1}{(l+n+1)^2} - \frac{1}{(l+n)^2} \right]
$$
 (49)

in such a way that

$$
\epsilon_n = \sum_{m=0}^n \epsilon_0^{(m)} = \frac{\alpha^2}{8(l+n+1)^2} \ . \tag{50}
$$

The corresponding wave functions can be directly written from Eqs. (44), (26), and (27).

VI. CONCLUSIONS

In this work we have shown that the Schrödinger equation

$$
\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi_n(x)=\epsilon_n\psi_n(x)
$$

is equivalent to the Ricatti succession (24), with the spectrum given by (25) and the Hilbert space (26).

Furthermore, given a Hamiltonian $H^{(0)}$, we have defined a sequence of Hamiltonians $\{H^{(n)}\}\$, in such a way that each one has the same spectrum as the preceding one, except the ground state, and with the Hilbert spaces connected by the operators $A^{(m)}$ and $A^{(r)}$

$$
\psi_m^{(n)} \sim A^{(n)^{\dagger}} \psi_{m-1}^{(n+1)},
$$

$$
\psi_m^{(n+1)} \sim A^{(n)} \psi_{m+1}^{(n)},
$$

according to Eqs. (14) and (15). This in fact conforms to a sequential approach to solve the Schrodinger equation in which we use at all levels nodeless wave functions, simply related with the actual ones.

If it is necessary or convenient, we can of course implement a perturbative approach from Eqs. (24), using the appropriate techniques for Ricatti equations.⁶ An example of a variational application is given in Ref. 2 for the first excited state of the anharmonic oscillator. Here we have shown that these procedures can be implemented without difficulty for any level in a sequential way beginning with the ground state.

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