The variational method in quantum mechanics: an elementary introduction

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Abstract

Variational methods in quantum mechanics are customarily presented as invaluable techniques to find approximate estimates of ground state energies. In the present paper a short catalogue of different celebrated potential distributions (both 1D and 3D), for which an exact and complete (energy and wavefunction) ground state determination can be achieved in an elementary way, is illustrated. No previous knowledge of calculus of variations is required. Rather, in all presented cases the exact energy functional minimization is achieved by using only a couple of simple mathematical tricks: ‘completion of square’ and integration by parts. This makes our approach particularly suitable for undergraduates. Moreover, the key role played by particle localization is emphasized through the entire analysis. This gentle introduction to the variational method could also be potentially attractive for more expert students as a possible elementary route toward a rather advanced topic on quantum mechanics: the factorization method. Such an unexpected connection is outlined in the final part of the paper.

Keywords: quantum mechanics, education, variational methods

1. Introduction

Teaching quantum mechanics at an introductory (undergraduate) level is an ambitious but fundamental didactical mission. It is well known that the study of quantum mechanics poses

1 To Franco Gori, on his eightieth birthday.
such challenging math problems which often may obscure the physics of the concepts to be developed. The need to avoid, as much as possible, the use of mathematical equipment that could not be still present within the toolbox of undergraduates necessarily limits the number of topics to be offered with an adequate level of detail. Consider that even in the probably best introduction to quantum mechanics, namely the fourth volume of the celebrated 1970 Berkeley’s Physics course [1], it is explicitly stated that no rigorous approaches to solve Schrödinger’s equation are attempted.

Heisenberg’s uncertainty principle is the essence of quantum mechanics. Some important consequences of the uncertainty principle can be quantitatively appreciated simply by exploring the way the spatial confinement of a particle influences the possible values its energy can attain. In particular, spatial localization unavoidably implies the energy to be lower bounded. While this fact is evident for a particle in an infinite well (where the energy bound directly follows from boundary conditions), for the harmonic oscillator such a connection already turns out to be much less transparent. As a matter of fact, it could result in being somewhat puzzling, for nonexpert students, to grasp why the oscillator zero-point energy value $\hbar \omega / 2$ should follow from the sole spatial localization. The need to keep the math at a reasonably low level led me to a rather simple way to determine the full energy spectrum of the quantum harmonic oscillator [2]. The variational method was the key ingredient for achieving such a result.

It is well known that quantum mechanics can be formulated in an elegant and appealing way starting from variational first principles. One of the most important byproducts of such an approach is the variational method. In all introductory quantum mechanics textbooks, it is customarily presented as an invaluable technique aimed at finding approximate estimates of ground state energies [3–7]. However, in [2] the variational method has been used in a rather unusual way to find, with only a few elements of basic calculus, the complete (energy and wavefunction) ground state of the harmonic oscillator, without any additional assumptions but wavefunction square integrability, which is the mathematical translation of the spatial confinement requirement. It is natural to wonder whether the approach used in [2] is limited to the particularly simple mathematical structure of the harmonic oscillator potential or if it has a wider applicability.

This is the principal aim of the present paper: to provide a gentle, as elementary as possible introduction to variational methods in quantum mechanics. To this end, we will illustrate a short ‘catalogue’ of several celebrated potential distributions for which the ground state can be found without actually solving the corresponding Schrödinger equation, but rather through a direct minimization of an energy functional. Only the ground states will be considered here, as the corresponding minimization procedure can be carried out in an elementary way. The knowledge of higher-order eigenstates would require mathematical techniques that are out of the limits and the scopes of the present paper. The work is organized in the form of a self-contained didactical unit. In section 2 the 1D stationary Schrödinger equation and the variational method are briefly recalled, together with the main results of [2]. In this way, the elementary character of the derivation will appear. Subsequently, three celebrated examples of potentials will be examined from the same variational point of view in order to show how their ground states can be characterized in a way accessible to any undergraduate. Two of these potentials are one-dimensional (1D henceforth), precisely the Morse and the Pöschl-Teller potentials. They will be examined in section 3 and in section 4, respectively. A fundamental three-dimensional (3D henceforth) problem, namely the determination of the hydrogen atom ground state, will also be presented in section 5. In all above
examples the minimization of the energy functional is achieved with the help of only two mathematical tricks: the so-called ‘square completion’ and the integration by parts, that should be part of the background of first-year Physics or Engineering students. But there is more.

During the minimization process, the starting energy functional is reduced to the sum of two terms: the first is the energy bound, the second is a nonnegative functional that vanishes when the wavefunction is the solution of a suitable first order linear ordinary differential equation, which can be solved again with elementary math tools (variable separation). In the final part of the paper (section 6) it will be shown how the procedure just described could be part of a possible elementary introduction to the so-called factorization method. Factorization was introduced at the dawn of quantum mechanics by Schrödinger and by Dirac as a powerful algebraic method to obtain the complete energy spectrum of several 1D quantum systems. It will be shown that the approach pursued throughout the present paper provides a didactically effective way to derive several examples of exact factorizations. We are not aware of previous attempts aimed at providing a variational route to factorization. Accordingly, such a direct connection could also be offered to more expert audiences (graduate students) who would benefit from the present derivation to better appreciate the elegance and powerfulness of the variational language.

2. Preliminaries

Consider the 1D motion of a mass point \( m \) under the action of a conservative force which is described via the potential energy function \( U(x) \). Schrödinger’s equation for the stationary state \( u = u(x) \) reads

\[
\frac{-\hbar^2}{2m} \frac{d^2 u}{dx^2} + U(x) u = E \ u,
\]

where \( \hbar = h/2\pi \), \( h \) being Planck’s constant. All (real) solutions of equation (1) describing bound energy’s eigenstates must be square integrable on the whole real axis,

\[
\int_{-\infty}^{+\infty} u^2(x) dx < \infty.
\]

The ground state for the potential \( U(x) \) can be found, in principle, without explicitly solving equation (1). To this end, it is sufficient to multiply its left and right side by \( u \) and then integrate them over the whole real axis. After simple algebra we obtain

\[
E = \frac{\int U(x) u^2 \ dx - \frac{\hbar^2}{2m} \int u \ u'' \ dx}{\int u^2 \ dx},
\]

where it will be tacitly assumed henceforth that any integration has to be carried out across the whole real axis (\( -\infty, +\infty \)). Now partial integration is applied to the second integral in the numerator of equation (3), which transforms as follows:

\[
\int u \ u'' \ dx = -\int u'^2 \ dx,
\]

where use has been made of the spatial confinement condition in equation (2). Substitution from equation (4) into equation (3) gives
Equation (5) will be the starting point of our analysis. Before continuing, the teacher should advise his/her students that the quantity in the rhs of equation (5) is a mathematical object called functional and that the branch on mathematics that studies the properties of functionals, the calculus of variations, is a rather advanced topic. Functional minimization requires the knowledge of mathematical techniques that cannot be part of undergraduate backgrounds. On the other hand, elementary derivations of Schrödinger’s equation solutions constitute exceptions rather than the rule. As a consequence, the number of quantum systems that can be adequately studied with a limited use of math is considerably small. In [2] it was shown that the energy functional in equation (5) can be minimized in an elementary way for the special case of the harmonic oscillator. The main result found in [2] will now be briefly resumed. This would help to clarify how the minimization of the energy functional (5) can be carried out, in some fortunate cases, by using only ‘completion of square’ and integration by parts.

Consider then a harmonic oscillator with frequency $\omega$, whose potential energy is

$$U(x) = \frac{1}{2}m\omega x^2.$$  

It is useful to introduce ‘natural units’ for length and energy in order for the functional (5), as well as the corresponding Schrödinger equation, to be reduced to dimensionless forms. Here and in the rest of the lecture this will be achieved by suitably combining the physical parameters of the specific problem and Planck’s constant. For the harmonic potential two natural units are the quantities $\sqrt{\hbar/m\omega}$ and $\hbar\omega/2$ for length and energy, respectively. In this way, equation (5) takes on the following form:

$$E = \frac{\int [\frac{\hbar^2}{2m}u'^2 + U(x)u^2] \, dx}{\int u^2 \, dx}.$$  

To minimize the rhs of equation (7), the square in the numerator is first completed, which yields

$$\int (u'^2 + x^2 u^2) \, dx = \int (u' + x u)^2 \, dx - 2 \int x \, u \, u' \, dx,$$

then a partial integration is performed on the last integral. In particular, on taking equation (2) into account, we have

$$-2 \int x \, u \, u' \, dx = \int u^2 \, dx,$$

so that, after simple algebra, equation (7) becomes [2]

$$E = \frac{\int (u' + xu)^2 \, dx}{\int u^2 \, dx} + 1.$$  

From equation (10) it follows that the oscillator energy cannot assume values less than $\hbar\omega/2$ (when expressed through physical units). Moreover, from the above analysis it is also evident how the localization constraint in equation (2) is solely responsible for the above energy.

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1 To avoid symbol proliferation, the same notations will be used to denote physical as well as dimensionless quantities.
bound. This is in perfect agreement with Heisenberg’s uncertainty principle. But there is more.

From equation (10) it also follows that, in order for the oscillator energy bound to be attained, the wavefunction must satisfy the following first order linear differential equation:

$$u'' + xu = 0,$$  \hspace{1cm} (11)

whose general integral, that can be found with elementary tools (variable separation), is the well known Gaussian function

$$u(x) \propto \exp\left(-\frac{x^2}{2}\right).$$ \hspace{1cm} (12)

Before continuing, it must be stressed once again how the above results have been obtained, after all, by imposing solely the localization constraint (2) on the energy functional (7). In the next section the same procedure will be used to find the ground state of the Morse oscillator.

3. Morse potential

The celebrated Morse potential, described by the two-parameter function

$$U(x) = U_0 [\exp(-2kx) - 2 \exp(-kx)],$$ \hspace{1cm} (13)

was proposed in 1929 by Morse [8] as a simple analytical model for describing the vibrational motion of diatomic molecules. Considerably accurate descriptions of vibrational spectra of several diatomic molecules have been obtained starting from the knowledge of Morse’s energy spectrum. Although the eigensolutions of the Schrödinger equation for the potential (13) are out of the scope of any introductory course on quantum mechanics, the exact determination of the ground state of the Morse oscillator can be achieved via the procedure outlined in the previous section.

In figure 1 a graphical representation of the Morse potential is sketched. It appears that quantities $k^{-1}$ and $U_0$ provide natural units for length and energy, respectively. Accordingly, on using the transformations $kx \rightarrow x$ and $E/U_0 \rightarrow E$, it is immediately proved that the energy functional (5) becomes
\[ E = \frac{\int \{ \alpha^2 u'^2 + u^2 [\exp(-2x) - 2 \exp(-x)] \} \, dx}{\int u^2 \, dx}, \quad (14) \]

the dimensionless parameter \( \alpha \) being defined by

\[ \alpha = \frac{\hbar k}{\sqrt{2mU_0}}. \quad (15) \]

Moreover, on further letting \( x \to \alpha x \), after simple algebra equation (14) can be recast as follows:

\[ E = \frac{\int \{ u'^2 + u^2 [1 - \exp(-\alpha x)]^2 \} \, dx}{\int u^2 \, dx} - 1. \quad (16) \]

To minimize the functional (16), the square into the integral in the numerator will first be completed. To this end, let the integral be recast as follows:

\[
\int \{ u'^2 + u^2 [1 - \exp(-\alpha x)]^2 \} \, dx = \int \{ u' + [1 - \exp(-\alpha x) + \chi] u \}^2 \, dx + \epsilon \int u^2 \, dx, \quad (17)
\]

then search those values of \( \chi \) and \( \epsilon \) for equation (17) to be satisfied. The first integral into the rhs of equation (17) is expanded to have

\[
\int \{ u' + [1 - \exp(-\alpha x) + \chi] u \}^2 \, dx = \int \{ u'^2 + u^2 [1 - \exp(-\alpha x) + \chi^2] \} \, dx + 2 \int uu' [1 - \exp(-\alpha x) + \chi] \, dx.
\]

(18)

Then, partial integration is applied to the last integral,

\[ 2 \int uu' [1 - \exp(-\alpha x) + \chi] \, dx = -\alpha \int u^2 \exp(-\alpha x) \, dx, \quad (19) \]

so that, after substitution into equation (18), simple algebra gives

\[
\int \{ u' + [1 - \exp(-\alpha x) + \chi] u \}^2 \, dx = \int \{ u'^2 + u^2 [1 - \exp(-\alpha x)] \} \, dx
\]

\[ + (\alpha^2 + 2\chi) \int u^2 \, dx - (\alpha + 2\chi) \int \exp(-\alpha x) u^2 \, dx. \quad (20) \]

On comparing equations (20) and (17) it is then found that \( \chi = -\alpha/2 \), so that \( \epsilon = -(\chi^2 + 2\chi) = \alpha - \alpha^2/4 \). Accordingly, equation (16) eventually becomes

\[ E = \frac{\int \left[ u' + \left(1 - \frac{\alpha}{2} - \exp(-\alpha x) \right) u \right]^2 \, dx}{\int u^2 \, dx} - \left(1 - \frac{\alpha}{2} \right)^2. \quad (21) \]

equation (21), when compared to equation (16), is considerably more informative. The true Morse oscillator energy lower bound is \(-1 - (\alpha/2)^2\). Moreover, to identify such a bound with the ground state energy, it is necessary to solve the following differential equation:

\[ u' + \left(1 - \frac{\alpha}{2} - \exp(-\alpha x) \right) u = 0, \quad (22) \]
which, by again using variable separation, gives at once

\[ u(x) \propto \exp \left[ -\left(1 - \frac{\alpha}{2}\right)x \right] \exp \left[ -\frac{1}{\alpha} \exp(-\alpha x) \right]. \tag{23} \]

Note that, in order for the function in equation (23) to represent a valid state, it is necessary that the arguments of both exponentials be negative, which occurs only if \( \alpha < 2 \), i.e. if the following condition:

\[ \frac{\hbar k}{\sqrt{2mU_0}} < 2, \tag{24} \]

is fulfilled.

It could be worth proposing to students an intuitive interpretation of the inequality (24), which I took from an exercise in the Berkeley textbook [1]. This should help students to appreciate how some basic features of a phenomenon can sometimes be grasped even by using idealized, nonrealistic models. Consider then the potential profile sketched as a dashed line in figure 2, where the left barrier is supposed to be infinitely high.

The parameter \( a \), that fixes the length scale, is expected to be proportional to \( k^{-1} \). It is a trivial exercise to find that the wavefunction describing the ground state of the step-like potential of figure 2 is, for \( 0 \leq x \leq a \),

\[ u(x) \propto \sin \left( \frac{\sqrt{2mE_0}}{\hbar} x \right), \quad 0 \leq x \leq a, \tag{25} \]

with \( E_0 < U_0 \) being the ground state energy. For \( x > a \), the wavefunction \( u(x) \) turns out to be

\[ u(x) \propto \exp \left[ -\frac{\sqrt{2m(U_0 - E_0)}}{\hbar} x \right], \quad x > a. \tag{26} \]

Since \( u(x) \) must be, together with its first derivative, continuous everywhere, it is necessary for the derivative of the sinusoidal function in equation (25) at \( x = a \) to be negative, thus implying

\[ \frac{\hbar k}{\sqrt{2mU_0}} < 2. \]
Moreover, since $E_0$ is less than $U_0$, from equation (27) it also follows that

$$\frac{\sqrt{2mE_0}}{\hbar} a > \frac{\pi}{2}. \tag{27}$$

formally identical to the inequality in equation (24) once letting $k \sim \pi/a$.

Before concluding the present section it is worth giving a simple but really important example of what kind of information could be, in some cases, obtained by only the ground state knowledge. To this end, consider its value measured with respect to the bottom of the potential curve, which is (in terms of the above defined dimensionless units) $\alpha = 2/4$. On coming back to physical units and on taking equation (15) into account, the ground energy is

$$\frac{\hbar}{2} \sqrt{\frac{2U_0 k^2}{m}} - \frac{\hbar^2 k^2}{8m}. \tag{29}$$

Note that the first term in equation (29) does coincide with the ground state energy of the harmonic approximation of the Morse potential (13), as can be easily proved by taking the second derivative of the potential at $x = 0$. Accordingly, the second term in equation (29) should be viewed as a quadratic (with respect to the parameter $hk$) anharmonic correction. If $\alpha$ were sufficiently small, it could then be possible to use the harmonic approximation to grasp information about, for instance, the vibrational spectrum of diatomic molecules\(^3\). To this end, Morse’s potential of equation (13) is used to fit the values of the interaction potential energy corresponding to the ground state of the hydrogen molecule, which have been accurately computed, for instance, by Kolos and Wolniewicz [10]. This is shown in figure 3, where the dashed curve contains the KW values, while the solid curve gives the behaviour of Morse’s

\(^3\) A beautiful, didactically speaking, introduction to vibrational spectra of diatomic molecules can still be found on the Berkeley textbook [1].
potential for $U_0 \approx 4.7$ eV and $k \approx 2.0$ Å$^{-1}$. Then, on identifying $m = m_p/2$ as the reduced mass of the H$_2$ molecules, equation (13) gives at once $\alpha \approx 0.06$. Such a small value would justify the above harmonic approximation of the ground state tone, which turns out to be about 4500 cm$^{-1}$, in agreement with its experimental value [11]$^4$.

4. Pöschl-Teller potential

The second case we are going to deal with is the so-called Pöschl-Teller potential, defined as follows:

$$U(x) = -\frac{U_0}{\cosh^2 kx}$$  \hspace{1cm} (30)

It is a useful analytical model to describe finite potential wells as well as anharmonic oscillators, and is sketched in figure 4.

Similarly to what was done for Morse’s potential, to find the ground state of the Pöschl-Teller potential (30), the dimensionless parameter $\alpha$ defined in equation (15) is first introduced, i.e. lengths and energies will again be measured in terms of $U_0$ and $\alpha/k$, respectively. In this way it is easy to prove that equation (5) reduces to

$$E = \frac{\int (u'^2 - \frac{u^2}{\cosh^2 \alpha x})dx}{\int u^2 dx}.$$  \hspace{1cm} (31)

Before proceeding to the minimization, it is better to recast equation (31) as follows:

$$E = \frac{\int (u'^2 + u^2 \tanh^2 \alpha x)dx}{\int u^2 dx} - 1,$$  \hspace{1cm} (32)

which implies that the energy must be greater than $-1$ ($-U_0$ in physical units), as can be inferred from figure 4. To obtain the true energy lower bound, the square inside the integral into the numerator of equation (32) has to be completed. To this end, we shall let

$^4$ Rigorously speaking, to identify the internuclear distance by the $x$ variable of equation (13) would imply the inclusion of an unphysical region corresponding to negative values of the internuclear distance. However, it was pointed out how such inclusion does not dramatically alter the resulting vibrational spectrum [8].

$^5$ Actually the potential in equation (30) is customarily named hyperbolic Pöschl-Teller potential, and was first considered by Eckart as a simple continuous model to study the penetration features of some potential barriers [9].
\[ \int (u'^2 + u^2 \tanh^2 \alpha x) dx = \int (u' + \chi u \tanh \alpha x)^2 dx + \epsilon \int u^2 dx, \] (33)
and then search for the values of \( \chi \) and \( \epsilon \) such that equation (33) is fulfilled. The first integral in the rhs of equation (33) is expanded as
\[ \int (u' + \chi u \tanh \alpha x)^2 dx = \int (u'^2 + \chi^2 u^2 \tanh^2 \alpha x) dx + 2\chi \int \tanh \alpha x u u' dx. \] (34)
Partial integration is then applied to the second integral in the rhs of equation (34),
\[ 2\chi \int \tanh \alpha x u u' dx = -\alpha \chi \int \frac{u^2}{\cosh^2 \alpha x} dx = \alpha \chi \int (\tanh^2 \alpha x - 1) u^2 dx. \] (35)
Finally, on substituting from equation (35) into equation (34), long but straightforward algebra gives
\[ \int (u' + \chi u \tanh \alpha x)^2 dx = \int [u'^2 + (\alpha \chi + \chi^2) u^2 \tanh^2 \alpha x] dx - \alpha \chi \int u^2 dx, \] (36)
which turns out to be identical to equation (33) when \( \chi \) coincides with the positive solution of the algebraic equation\(^6\)
\[ \alpha \chi + \chi^2 = 1. \] (37)
With such a choice in mind and on taking into account that \( \epsilon = -\alpha \chi \), equation (36) can be substituted into equation (32), which takes on the form
\[ E = \frac{\int (u' + \chi u \tanh \alpha x)^2 dx}{\int u^2 dx} - \chi^2. \] (38)
It then follows that the ground state energy of the Morse oscillator is just \(-\chi^2\), with the corresponding wavefunction being the solution of the following differential equation:
\[ u' + \chi u \tanh \alpha x = 0. \] (39)
On again using variable separation, it is immediately found that
\[ u(x) \propto \cosh^{-s} \alpha x, \] (40)
where
\[ s = \frac{1}{2} \left( \sqrt{1 + \frac{4}{\alpha^2}} - 1 \right). \] (41)
It should be noted that the result obtained for the Pöschl-Teller potential could be, in principle, extended to deal with other important 1D models. Students should be encouraged to study, for instance, the so-called Rosen-Morse potential, defined by [12]
\[ U(x) = -U_0 \left( \frac{1}{\cosh^2 kx} - 2\eta \tanh kx \right), \] (42)
where \( \eta \in (-1, 1) \). The Rosen-Morse potential, originally proposed as a simple analytical model to study the energy levels of the NH\(_3\) molecule, can be viewed as a modification of the Pöschl-Teller potential in which the term \(-2\eta \tanh kx\) allows the asymptotic limits for \( x \to \pm \infty \) to split, as can be appreciated by looking at figure 5, where a pictorial
\[^6\] Equation (37) is the reason why the Pöschl-Teller potential (30) is often written in the equivalent form
\[ U(x) = \frac{\hbar^2 k^2}{2m} \frac{s(s + 1)}{\cosh^2 kx}, \]
where \( s = \chi/\alpha \).
representation of the potential (42) has been sketched. Some hints aimed at guiding students to find the ground state of the Rosen-Morse potential are given in the appendix.

5. Hydrogen atom

The final example we wish to offer is a simple and compact determination of the ground state of the hydrogen atom. Schrödinger’s equation for the electron wavefunction within the Coulomb electric field produced by the nucleus is first recalled,

$$-\frac{\hbar^2}{2m} \nabla^2 u - \frac{e^2}{r} u = E u,$$

where \(\nabla^2(\cdot)\) denotes the Laplacian operator acting on the stationary states \(u = u(r)\), with \(r\) denoting the electron position vector with respect to the nucleus. Since the Coulombian potential depends only on the radial distance \(r = |r|\), Schrödinger’s equation (43) is customarily written by using spherical coordinates \((r, \theta, \phi)\) as follows:

$$-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2 (ru)}{\partial r^2} + \frac{1}{2mr^2} \hat{L}^2 u - \frac{e^2}{r} u = E u,$$

where the differential operator \(\hat{L}^2\), acting only on the angular variables \((\theta, \phi)\), corresponds to the squared modulus of the angular momentum. The presence of the term \(\hat{L}^2/2mr^2\) into the Hamiltonian implies that the eigenvalues \(E\) will contain an amount of (positive) energy which has to be ascribed to the presence of centrifugal forces that tend to repel the electron from the force centre. For this reason the ground state, i.e. that having the minimum energy, will be an eigenstate of \(\hat{L}^2\) corresponding to a null value of angular momentum. In other words, only radially symmetric wavefunctions, i.e. \(u = u(r)\), will be considered into equation (44).

Moreover, on using Bohr’s radius \(a_B = \hbar^2/m\varepsilon_0^2\) and the hydrogen ionization energy \(\varepsilon_0 = me^4/2\hbar^2\) as unit length and unit energy, respectively, it is possible to recast equation (44) as follows:

$$-\frac{1}{r^2}(r^2u')' - \frac{2u}{r} = E u.$$

Figure 5. A pictorial representation of the Rosen-Morse potential in equation (42).
Similarly as was done for the 1D cases, we multiply both sides of equation (45) by \( u(r) \) and then integrate over the whole 3D space\(^7\). After simple algebra the corresponding energy functional is then obtained,

\[
E = -\int u(r^2 u') \, dr + 2 \int u^2 r \, dr, \tag{46}
\]

where it will now be assumed henceforth that the limits of \( r \)-integrals are \([0, \infty)\). Partial integration in both integrals into the numerator gives

\[
E = \frac{\int (u'^2 + 2 uu') r^2 \, dr}{\int u^2 r^2 \, dr}. \tag{47}
\]

Then, on completing the square, i.e.

\[
\int (u'^2 + 2 uu') r^2 \, dr = \int (u' + u)^2 r^2 \, dr = \int u^2 r^2 \, dr,
\]

equation (47) eventually becomes

\[
E = \frac{\int (u' + u)^2 r^2 \, dr}{\int u^2 r^2 \, dr} - 1, \tag{49}
\]

from which it follows that the hydrogen ground energy is \(-\mathcal{E}_0\). From equation (49) it also follows that the ground state wavefunction must be the solution of the differential equation

\[
u' + u = 0, \tag{50}
\]

i.e. it is proportional to the well known radial function \(\exp(-r/a_B)\).

6. A possible elementary route to factorization?

What has been shown so far is enough to cover at least two didactical units (lecture and recitation session). Nevertheless, in the present section we would offer teachers a way to introduce, again by using only elementary tools, a rather advanced topic of quantum mechanics, the so-called factorization method, introduced during the early days of quantum mechanics as a powerful algebraic method to solve stationary Schrödinger’s equations\([13–16]\).

A possible elementary introduction to factorization could start again from the analysis of the harmonic oscillator potential recalled in section 2. Schrödinger’s equation, expressed via the above introduced “natural units,” reads

\[
u'' + x^2 u = E u. \tag{51}
\]

Consider then equation (11), which will be recast in the following form:

\[
\left( \frac{d}{dx} + x \right) u = 0, \tag{52}
\]

\(^7\) For radial functions the 3D integration reduces to a 1D integration,

\[
\int_{0}^{\infty} r^2 \, dr = 4\pi \int_{0}^{\infty} r^2 \, dr.
\]
whose lhs can be interpreted in terms of the action of the differential operator \( x + \frac{d}{dx} \) on the ground state wavefunction \( u(x) \). Equation (52) gives an implicit, although complete characterization of the harmonic oscillator ground state. In other words, from equation (52) it is possible not only to retrieve the ground state wavefunction \( u(x) \), as it was done before, but also the corresponding value of the ground state energy. To this end, consider the following differential operator:

\[
\left( -\frac{d}{dx} + x \right) \left( \frac{d}{dx} + x \right).
\]  

(53)

where the first ‘factor’ has been obtained simply by changing the sign of the derivative operator \( \frac{d}{dx} \) within the factor of equation (52). In this way, the operator in equation (53) turns out to be Hermitian. Moreover, on using solely the Leibniz differentiation rule for the product, it is a trivial exercise to expand the operator in equation (53) as follows:

\[
\left( -\frac{d}{dx} + x \right) \left( \frac{d}{dx} + x \right) = -\frac{d^2}{dx^2} + x^2 - 1,
\]  

(54)

so that, after substitution into equation (51), the Schrödinger equation for the harmonic oscillator takes on the factorized form

\[
\left( -\frac{d}{dx} + x \right) \left( \frac{d}{dx} + x \right) u = (E - 1)u.
\]  

(55)

From equation (55), on again taking equation (52) into account, it follows that the energy of the ground state is just 1. Its characterization is complete, as promised.

As a further example, consider again the Morse potential of section 3. At the end of the functional minimization process, equation (21) has been obtained. Now, similarly as done for the harmonic oscillator, consider the following differential operator:

\[
\left( -\frac{d}{dx} + 1 - \frac{\alpha}{2} \exp(-\alpha x) \right) \left( \frac{d}{dx} + 1 - \frac{\alpha}{2} - \exp(-\alpha x) \right).
\]  

(56)

which, after expansion, takes on the form

\[
-\frac{d^2}{dx^2} + \left[ \exp(-2\alpha x) - 2 \exp(-\alpha x) \right] \left( 1 - \frac{\alpha}{2} \right)^2.
\]  

(57)

Then also the stationary Schrödinger equation of the Morse oscillator,

\[-u'' + \left[ \exp(-2\alpha x) - 2 \exp(-\alpha x) \right] u = E \ u,
\]  

(58)

takes a factorized form, precisely

\[
\left( -\frac{d}{dx} + 1 - \frac{\alpha}{2} \exp(-\alpha x) \right) \left( \frac{d}{dx} + 1 - \frac{\alpha}{2} - \exp(-\alpha x) \right) u
\]

\[
= \left[ E + \left( 1 - \frac{\alpha}{2} \right)^2 \right] u.
\]  

(59)

Students should be encouraged to prove that, starting from equation (38), the Schrödinger equation for the Pöschl-Teller potential (30) can also be factorized as
\[-\frac{d^2}{dx^2} + U(x)\]

with \(\chi\), of course, being the solution of equation (37). Similar considerations hold for the Rosen-Morse potential.

All above examples showed that the lhs of 1D Schrödinger’s equation can be written as the product of two first order differential operators plus a constant term. This is the essence of factorization: given the potential \(U(x)\), to find a function, say \(\beta(x)\), and a constant, say \(\epsilon\), such that the Hamiltonian operator

\[-\frac{d^2}{dx^2} + U(x)\]

can be expressed as

\[-\frac{d^2}{dx^2} + U(x) = \left[-\frac{d}{dx} + \beta(x)\right]\left[\frac{d}{dx} + \beta(x)\right] + \epsilon.\]

The general solution of the factorization problem requires advanced mathematical techniques, like the use of a nonlinear differential equation. Remarkably, such a differential equation can easily be derived by using the variational approach used throughout the whole paper. To this end, consider the energy functional (5) written in terms of suitable dimensionless quantities,

\[E = \frac{\int [u'^2 + U(x)u^2] dx}{\int u^2 dx}.\]

For what it was said, it should be desirable to recast equation (63) as

\[E = \frac{\int [u'^2 + (\beta(x))u^2 + \epsilon u^2] dx}{\int u^2 dx} + \epsilon,\]

or, after rearranging and expanding, as

\[E = \frac{\int [u'^2 + \beta^2(x)u^2 + \epsilon u^2] dx + 2 \int \beta(x)uu'dx}{\int u^2 dx}.\]

Then, on evaluating the second integral in the numerator of equation (65) again by parts, i.e.

\[2 \int \beta(x)uu'dx = -\int \beta'(x)u^2dx,\]

equation (65) eventually becomes

\[E = \frac{\int \{u'^2 + \beta^2(x) - \beta'(x) + \epsilon \} u^2 dx}{\int u^2 dx},\]

which does coincide with equation (64) only if \(\beta(x)\) and \(\epsilon\) satisfy the Riccati-type differential equation

\[\beta^2(x) - \beta'(x) + \epsilon = U(x).\]

It is easy to prove that the same differential equation is also obtained by expanding the rhs of equation (62), thus completing our elementary proof. Students can be invited to check equation (68) for the entire catalogue presented here. It should be pointed out how exact

As usual, suitable units for length and energy are used to make the corresponding Schrödinger equation dimensionless.
solutions of the Riccati equation (68) can be derived via a purely algebraic way, starting from a simple minimum principle.

In a monumental review paper published at the very beginning of the fifties [17], Infeld and Hull presented a systematic study about all possible 1D potentials for which the corresponding stationary Schrödinger equation can be exactly factorized. Some of them have been analyzed here. It could also be worth exploring the Infeld/Hull catalogue to find, and certainly there are, other interesting cases to study. In this way even graduate students could benefit from our elementary derivation to better appreciate the power and the elegance of the variational language.

Appendix. Ground state of Rosen-Morse potential

In the present section, some hints are given to help students reaching the ground state of the potential into equation (42). The starting point is, needless to say, the energy functional that, on taking equation (42) into account, can be recast as follows:

\[ E = \frac{\int [u'^2 + (\alpha + \eta)^2 u^2] \, dx}{\int u^2 \, dx} - (1 + \eta^2), \quad (A.1) \]

where the symbol \( \alpha \) stands for \( \tanh \alpha x \), \( \alpha \) being defined again by equation (15). Similarly as was done for the Pöschl-Teller, the integral into the numerator of equation (A.1) is written as a perfect square. To this end, the free parameters, \( \chi \), \( \beta \), and \( \epsilon \) are introduced, and their values are chosen in such a way that the following relation holds:

\[ \int [u'^2 + (\alpha + \eta)^2 u^2] \, dx = \int [u' + \chi (\alpha + \beta) u]^2 \, dx + \epsilon \int u^2 \, dx, \quad (A.2) \]

with \( \epsilon \) being a constant factor which contributes to the final expression of the ground state energy. On expanding both sides of equation (A.2), it is not difficult to show that the parameters \( \chi \), \( \beta \), and \( \epsilon \) must satisfy the following algebraic relationships:

\[
\begin{cases}
\chi^2 + \alpha \chi = 1, \\
\chi^2 \beta = \eta, \\
\epsilon = \eta^2 - \chi^2 \beta^2 + \alpha \chi.
\end{cases} \quad (A.3)
\]

Note that the first of the above equations coincides with equation (37). Then, on inserting from equation (A.2) into equation (A.1) and on taking equation (A.3) into account, simple algebra gives

\[ E = \frac{\int [u' \chi (\alpha + \beta) u] \, dx}{\int u^2 \, dx} - \chi^2 (1 + \beta^2), \quad (A.4) \]

from which the ground state follows.

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