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The envelope theory as a pedagogical tool

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Abstract

The envelope theory (ET) is a reliable and easy to implement method to solve time independent Schrödinger-like equations (eigenvalues and eigenvectors). It is particularly useful to solve many-body systems since the computational cost is independent from the number of particles. The purpose of this paper is twofold. First, we want to make known a method that is probably too little used. Second, we also want to show that this method can be used as a pedagogical tool, thanks to its simplicity and the reliable results that can be obtained. To reach these goals, the ET is applied to a simple problem in one dimension, the soft-Coulomb potential $-k/\sqrt{x^2+d^2}$, characterised by a bias distance d. Such interaction is used for the study of excitons, electron–hole bound pairs where the two charges are kept separated in two different one-dimensional regions (quantum wires). In addition to its physical interest, this system has never been treated with the ET.

Keywords: envelope theory, excitons, teaching of quantum mechanics

(Some figures may appear in colour only in the online journal)

1. Introduction

Finding the eigenvalues and eigenvectors of Hamiltonians is a fundamental problem in quantum mechanics. Various methods can be used as the variational one, the WKB approximation or the perturbation theory, for instance [1, 2]. All these methods rely on the construct of good approximations for the wavefunctions. The principle is different for the envelope theory (ET) in which the Hamiltonian under study H is approximated by an 'auxiliary Hamiltonian' $\tilde{H}$ which depends on 'auxiliary parameters' and whose solutions are exactly known [3–6]. These auxiliary parameters are determined by an extremisation procedure applied to the eigenvalues of the auxiliary Hamiltonian. The eigenvalues and

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eigenvectors of the optimised $\tilde{H}$ are then the approximate solutions of H. A practical choice for $\tilde{H}$ is a harmonic oscillator Hamiltonian. Even if the accuracy is not great, the method is reliable and analytical upper or lower bounds can be obtained in favourable situations. The ET is mainly useful for many-body systems since the computational cost is independent from the number of particles, but it can also be used as a pedagogical tool as it is very easy to implement and allows the computation of the whole spectrum.

In this paper, the ET is applied to the study of the soft-Coulomb potential $-k/\sqrt{x^2+d^2}$ in one dimension, characterised by a bias distance d. This interaction is chosen for three reasons: (i) it has a great physical interest since it is characteristic of excitons, electron–hole bound pairs where the two charges are kept separated in two different one-dimensional regions. These systems, named quantum wires, appear in solid state physics [7] and in various biological processes [8]; (ii) it is bounded from below and from above by two potentials for which known exact solutions can be used as control lower and upper bounds; (iii) it is studied in a recent paper by the variational method [9] which allows interesting comparisons.

The recipe to use the ET for a two-body system in one dimension is presented in section 2, where some justifications about the relevance of the method are given. The ET is applied to the one-dimensional soft-Coulomb potential $-k/\sqrt{x^2+d^2}$ in section 3, where eigenvalues and eigenvectors are computed and compared with results coming from accurate numerical calculations and from a variational method. Concluding remarks are given in section 4 where some suggestions for the use of the ET as a pedagogical tool are proposed.

2. The envelope theory

In this section, matters from several papers [5, 10, 11] are collected and summarised to describe how to compute the approximate ET solutions for the generic one-dimensional Hamiltonian given by

$$H = T(\hat{p}) + V(x), \tag{1}$$

where x is a position variable, $\hat{p} = -\mathrm{i}\hbar\mathrm{d}/\mathrm{d}x$ the momentum conjugated with x, T the kinetic term and V the potential. In the following, it is necessary to make the difference between the momentum as an operator, denoted by $\hat{p}$, and the momentum as a simple variable, denoted by p. The domain of x can be $\mathbb{R}_+$ or $\mathbb{R}$. In this last case, V is an even function of x for physical and practical reasons. T is always expected to be an even function of p [12]. The approximate energy E for the nth level is given by an extremisation procedure of the corresponding eigenvalue of the associated auxiliary Hamiltonian $\tilde{H}$. But it can be shown that it is equivalent to solve the following system for each value of the quantum number n

$$E = T(p_0) + V(x_0), \tag{2}$$

$$x_0 p_0 = Q_n \hbar, \tag{3}$$

$$p_0 T'(p_0) = x_0 V'(x_0), \tag{4}$$

where $X'(z) = \mathrm{d}X/\mathrm{d}z$, $x_0 > 0$, $p_0 > 0$ and Q_n is defined by

$$Q_n = n + \frac{1}{2} \quad \text{for} \quad x \in \mathbb{R}, \tag{5}$$

$$Q_{n_o} = n_o + \frac{1}{2} \quad \text{for} \quad x \in \mathbb{R}_+, \tag{6}$$

where $n = 0, 1, 2, 3, \ldots$ and $n_o = 2n + 1 = 1, 3, 5, 7, \ldots$ The restriction to odd numbers n_o insures that the wave function vanishes at $x = 0$. The structure of Q_n comes from the use of the one-dimensional harmonic oscillator Hamiltonian as the auxiliary Hamiltonian $\tilde{H}$. Consequently, the corresponding approximate ET eigenstate is a harmonic oscillator one. This state, denoted $|n\rangle$, is such that $\tilde{H}\ |n\rangle = E\ |n\rangle$. For $x \in \mathbb{R}$, it is written [2]

$$\langle x|n\rangle = \psi_n(x) = \left(\frac{\lambda^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\lambda x) \exp\left(-\lambda^2 x^2/2\right), \tag{7}$$

where H_n is an Hermite polynomial and $\lambda = \sqrt{Q_n}/x_0$. For $x \in \mathbb{R}_+$, $\psi_{n_o}(x)$ must be multiplied by $\sqrt{2}$ to keep the correct normalisation. It can be checked that the ET gives the exact solutions for a harmonic oscillator Hamiltonian.

The way to obtain the system (2)–(4), that we call 'compact equations of the ET', is quite long and tricky. In the next paragraph, we simply give the main ideas leading to the ET, but the full demonstration can be found in [13] for nonrelativistic and semirelativistic kinematics. The generalisation for arbitrary kinetic energy is presented in [5]. The special case of one-dimensional systems is treated in [10] and the inclusion of a special type of many-body forces is detailed in [14]. In this last reference, a summary of the calculations performed in [13] gives the main steps for the construction of the ET. More recently, the compact equations for two sets of different particles have also been computed [11].

The ET has been first developed by Hall in a series of papers (see for instance [3, 4]) and rediscovered later under the name of 'auxiliary field method' by a completely different approach than the one used by Hall [15]. Starting from a Hamiltonian H under study, it is possible to build another Hamiltonian H^* containing functions of the positions and the momenta of particles, named 'auxiliary fields', in such a way that the elimination of these functions from H^* by a variational principle gives back H. So H^* is as complicated as H to solve. The idea is to replace in H^* the functions by numbers, the auxiliary parameters, to build the auxiliary Hamiltonian $\tilde{H}$ which can be solved exactly. The ET approximations are obtained by demanding that the exact eigenenergies of $\tilde{H}$ be stationary with respect to these auxiliary parameters. It is then possible to show that the extremisation equations can be replaced by a compact set of equations easier to handle. Each level is associated with a particular optimised $\tilde{H}$ (see (10) and (11) below). The ET approximations for the eigenenergy and the eigenstate of the nth level of H are the nth eigenenergy and eigenstate of the corresponding optimised $\tilde{H}$.

It can be shown that

$$\langle n|x^2|n\rangle = x_0^2 \quad \text{and} \quad \langle n|\hat{p}^2|n\rangle = p_0^2. \tag{8}$$

So, p_0 can be interpreted as the mean momentum and x_0 as the mean characteristic distance for the state. The mean value of an observable $\hat{A}(x^2, \hat{p}^2)$, where the function A allows a Taylor expansion, can then be approximated by

$$\langle n|\hat{A}(x^2, \hat{p}^2)|n\rangle \approx A(x_0^2, p_0^2). \tag{9}$$

The physical quantities x_0 and p_0 appear in the compact equations giving the definition of the energy (2), the rule for the quantisation (3), and the equation of motion (4) as a transcendental equation. This last equation is nothing else that the quantum virial theorem [16]. These three relations allow to give a nice semi-classical interpretation of the ET [5, 14]. Nevertheless, the

ET is a full quantum method giving eigenvectors and eigenvalues. In natural units, $\hbar = 1$ in (3).

The structure of T is usually simpler that the one of V. That is the reason why it is generally more convenient to work in the configuration space. But the symmetry between the momentum and the position in the system (2)–(4) indicates that computations can be performed indifferently in the configuration space (x as the variable with $\hat{p} = -\mathrm{i}\hbar\mathrm{d}/\mathrm{d}x$) or in the momentum space (p as the variable with $\hat{x} = i\hbar\mathrm{d}/\mathrm{d}p$).

In the ET, for each level n, the kinetic part $T(p)$ and the potential part $V(x)$ are respectively 'enveloped' by the following tangent quadratic functions (see the example in section 3.3)

$$\tilde{T}(p) = T(p_0) + \frac{T'(p_0)}{2p_0}(p^2 - p_0^2), \tag{10}$$

$$\tilde{V}(x) = V(x_0) + \frac{V'(x_0)}{2x_0}(x^2 - x_0^2). \tag{11}$$

This is the origin of the name of the method [3, 4]. The enveloping functions are such that $\tilde{T}(\hat{p}) + \tilde{V}(x) = \tilde{H}$ which is the optimised auxiliary Hamiltonian for the nth level (p_0 and x_0 depend on n by the set of equations (2)–(4)). It can be checked from (8), (10) and (11) that $E = \langle n|\tilde{H}|n\rangle$. If $T(p)$ ($V(x)$) is quadratic, $\tilde{T}(p) = T(p)$ ($\tilde{V}(x) = V(x)$). It is also clear from (11) that $\tilde{V}(x_0) = V(x_0)$ and $\tilde{V}'(x_0) = V'(x_0)$. This means that $\tilde{V}$ and V are tangent at the point $x = x_0$. If there is only one contact point, $\tilde{V}$ is either totally above or totally below V. Thanks to (10), the situation is similar for $\tilde{T}$ and T. If T and V are both bounded from above (below) by $\tilde{T}$ and $\tilde{V}$, the ET approximations for eigenenergies are upper (lower) bounds, according to the comparison theorem [17]. A simple criterion for this has been found in [3, 4]. By defining the two functions $b_T(p^2) = T(p)$ and $b_V(x^2) = V(x)$, it can be shown that E is an upper (lower) bound of the genuine eigenvalue if b_T and b_V are both concave (convex) functions. If the second derivative is vanishing for one of these functions, the variational character is solely ruled by the convexity of the other one. It is easy to check that the situation $b_T'' = b_V'' = 0$ corresponds to the harmonic oscillator Hamiltonian for which the system (2)–(4) gives the exact solution. In other cases, the variational character of the solution cannot be guaranteed. Let us note that E has an analytical form for a large variety of Hamiltonians for arbitrary values of the dimension [10, 13, 18].

3. The exciton Hamiltonian

The Hamiltonian H_{eh} for the electron–hole pair, where the two charges are kept separated in two different one-dimensional regions by a bias distance d, is given by

$$H_{\mathrm{eh}} = \frac{\hat{p}^2}{2m} - \frac{k}{\sqrt{r^2 + d^2}}, \tag{12}$$

where r ($\in\mathbb{R}$) is the relative position between the electron and the hole, $\hat{p}$ the conjugate momentum, m the reduced mass of the pair and $k = e^2/(4\pi\epsilon_0\epsilon_r)$, with e the elementary electric charge, ϵ_0 the dielectric permittivity in vacuum and ϵ_r the relative dielectric permittivity of the material. As the potential in (12) is vanishing for $|r| \to \infty$, the eigenvalues of H_{eh} are the binding energies of the electron–hole pair for the different levels. The purpose of this paper is not to investigate in detail exciton physics, but it is worth mentioning that the computation of the threshold for photon absorption requires in addition the knowledge of the bulk semiconductor's band gap [19]. This is out of the scope of this work.

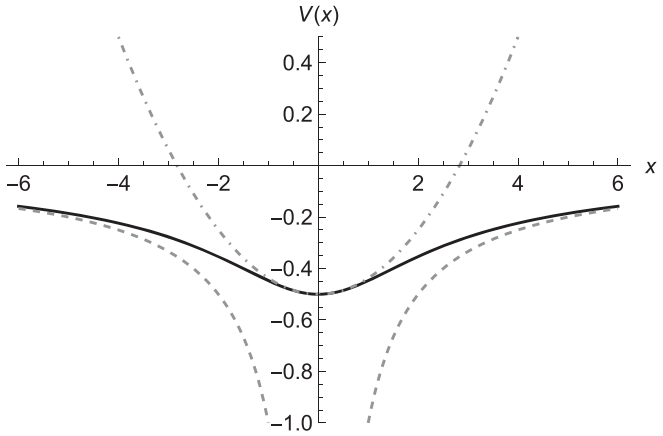

Figure 1. The soft-Coulomb potential for $D = 2$ (solid black) with the Coulomb potential (dashed gray) and the quadratic potential with $D = 2$ (dot-dashed gray). All quantities are dimensionless.

3.1. Dimensional analysis

It is always interesting to work with dimensionless variables in order to make apparent what are the relevant physical quantities and to simplify the formulation of the problem. By using the effective Bohr radius $a_{\mathrm{B}} = 4\pi\epsilon_0\epsilon_r\hbar^2/(me^2)$ and the effective Rydberg constant $\mathrm{R_y} = me^4/(32\pi^2\epsilon_0^2\epsilon_r^2\hbar^2) = k/(2a_{\mathrm{B}})$, a dimensionless Hamiltonian $H = H_{\mathrm{eh}}/(2\mathrm{R_y})$ can be defined in terms of a dimensionless bias parameter $D = d/a_{\mathrm{B}}$ and a dimensionless position $x = r/a_{\mathrm{B}}$

$$H = -\frac{1}{2}\frac{d^2}{\mathrm{d}x^2} - \frac{1}{\sqrt{x^2 + D^2}}, \tag{13}$$

whose dimensionless eigenvalues (binding energies) will be designed by E. Only dimensionless quantities will be used in the following. To recover physical quantities, x must be multiplied by a_{B} and E by $2\mathrm{R_y}$. Both a_{B} and $\mathrm{R_y}$ are pertinent units for contexts in which excitons appear. For instance, $a_{\mathrm{B}} = 16.34$ nm and $\mathrm{R_y} = 3.416$ meV for GaAs [9]. The standard range of d in typical GaAs-based devices is varied from 10 to 20 nm. So D is around unity for these semiconductors.

3.2. Bounding potentials

The soft-Coulomb potential $-1/\sqrt{x^2 + D^2}$ is bounded from below by the Coulomb potential $-1/|x|$ for $x \in \mathbb{R}$ (see figure 1). So, according to the comparison theorem, the eigenvalues of

$$H_{\mathrm{C}} = -\frac{1}{2}\frac{d^2}{\mathrm{d}x^2} - \frac{1}{|x|} \tag{14}$$

are lower bounds of the eigenvalues of H. The spectrum of H_{C} is analytical [20]

$$E_{\mathrm{C}} = -\frac{1}{2(n+1)^2}, \tag{15}$$

with $n = 0, 1, 2, 3, \ldots$ associated with wavefunctions vanishing at $x = 0$ and with $2n$ nodes at finite x values on $\mathbb{R}$. To correspond to our numbering scheme (5)–(6), (15) must be rewritten

$$E_{\mathrm{C}} = -\frac{2}{(n_{\mathrm{o}} + 1)^2}. \tag{16}$$

For large values of n_{o}, the eigenfunctions of H and H_{C} are characterised by a large extension, that is to say, a significant part in regions where both potentials are very similar. So it is expected that E and E_{C} will be very close in these situations.

An easy way to solve approximately a Schrödinger equation around an equilibrium point is to use a harmonic approximation of the potential. Expanding the soft-Coulomb potential in power of x around 0, H reduces to the harmonic oscillator Hamiltonian

$$H_{\mathrm{HO}} = -\frac{1}{2}\frac{d^2}{\mathrm{d}x^2} + \frac{x^2}{2D^3} - \frac{1}{D} \tag{17}$$

at the lowest order. The corresponding eigenvalues are given by [2]

$$E_{\mathrm{HO}} = \left(n + \frac{1}{2}\right)\frac{1}{D^{3/2}} - \frac{1}{D}. \tag{18}$$

It is easy to show that the quadratic potential in H_{HO} is always larger that the potential in H (see figure 1). So, according to the comparison theorem, E_{HO} are upper bounds of E. Moreover, both potentials are very similar for small values of x. It is then expected that E and E_{HO} will be very close for values of n close to 0, corresponding to eigenfunctions characterised by a small extension.

3.3. ET approximations

The ET solutions for H are computed by solving first (4), taking into account (3), with $\hbar = 1$ for nonrelativistic kinematics and the soft-Coulomb potential. With $T(p) = p^2/2$ and $V(x) = -(x^2 + D^2)^{-1/2}$, we have $T'(p) = p$ and $V'(x) = x(x^2 + D^2)^{-3/2}$. Injecting these results in (4), the equation for x_0 is then

$$x_0^4 = Q_n^2(x_0^2 + D^2)^{3/2}. \tag{19}$$

For given values of D and Q_n, analytical solution for x_0 can be written in terms of the solutions of a quartic equation, but the expression is so complicated that it is not usable in practice. Graphically, it is easy to check that (19) has only one positive solution for x_0^2. It is then very easy to compute it by a numerical procedure [21] or a software like Mathematica®. Once x_0 is computed, the ET approximation for the energy can be computed with (2) and (3). We have $b_T(p^2) = p^2/2$ and $b_V(x^2) = -(x^2 + D^2)^{-1/2}$. The ET approximations E_{ET} for the energies are upper bounds since $b_T''(z) = 0$ and $b_V(z) = -(z + D^2)^{-1/2}$ is a concave function. Finally, the ET upper bounds are given by

$$E_{\mathrm{ET}} = \frac{Q_n^2}{2x_0^2} - \frac{1}{\sqrt{x_0^2 + D^2}} \quad \text{with} \quad x_0^4 = Q_n^2(x_0^2 + D^2)^{3/2}. \tag{20}$$

As presented in section 3.2, the solutions for H must be close to the solutions for H_{C} and H_{HO} under certain conditions. Let us check this from (20). Provided D is not too large, it is expected from (19) that $x_0^4 \approx Q_n^2 x_0^3$, that is to say, $x_0 \approx Q_n^2$, when $n \gg 1$. In this case, the parameter D disappears in the dominant term and (20) reduces to

$$E_{\mathrm{ET}} \approx -\frac{2}{(2n + 1)^2}. \tag{21}$$

This last formula can be compared with E_{C} for odd values of n: (21) is clearly an upper bound of (16).

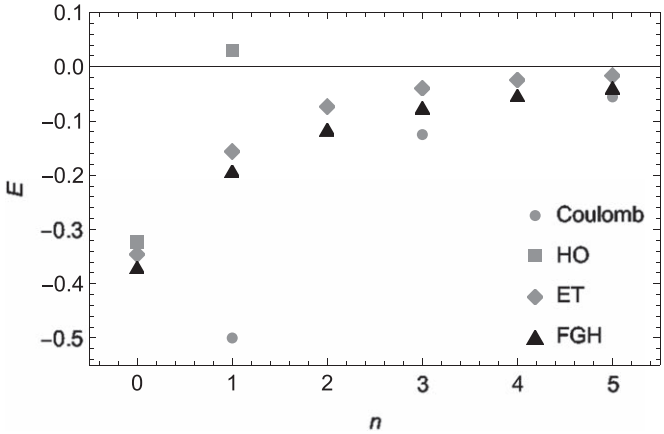

Figure 2. Lowest dimensionless energies for H with $D = 2$: accurate values obtained with the FGH method (black triangle) and upper bounds from the ET (gray diamond). The exact energies for H_{C} (gray circle) and H_{HO} with $D = 2$ (gray square) are also indicated.

If n is a small integer and D is not too small, an approximate solution for (19) is $x_0^4 \approx Q_n^2 D^3$, that is to say, $x_0^2 \approx Q_n D^{3/2}$. In this case, at the lowest order in n, (20) reduces to

$$E_{\mathrm{ET}} \approx \left(n + \frac{1}{2}\right)\frac{1}{D^{3/2}} - \frac{1}{D}, \tag{22}$$

which is identical to E_{HO}. This is not surprising since the ET gives the exact solutions for a harmonic oscillator Hamiltonian.

Accurate numerical eigenvalues and eigenvectors of H are computed with the Fourier Grid Hamiltonian (FGH) method [22, 23] which is very powerful and very easy to use for one-dimensional time-independent Schrödinger-like equations. In figure 2, these energies are compared with E_{ET} and the other bounds E_{HO} and E_{C}, for $D = 2$ and the lowest values of n. The ET approximations are good for all values of n. The lower bound E_{C} which is only defined for odd numbers n improves with increasing n, as expected. On the contrary, the upper bound E_{HO} degrades rapidly with increasing n, as expected also. It is worth drawing attention that the upper bounds E_{HO} are computed with a unique quadratic potential in (17) (see figure 1). The upper bounds E_{ET} are computed with a different envelope potential $\tilde{V}(x)$ for each value of n (see figure 3). Wavefunctions for the ground state and the first excited state, computed with the FGH method and the ET, are compared in figure 4 for three values of D. The agreement is good but the ET approximations decrease faster with x. This is due to the harmonic oscillator nature of the approximate wavefunctions which decrease as Gaussian functions while the exact solutions decrease as exponential functions.

3.4. Comparison with a variational method

The ground and first excited states of H have been computed in a recent paper by a variational method using the ground and first excited states of the harmonic oscillator Hamiltonian as trial states [9]. The results from this paper are compared with the ET results in figure 5 as a function of D. Let us mention that the dimensionless numbers obtained with the formulas in [9] must be divided by 2 to be compared with our results because the energies are given in unit of $\mathrm{R_y}$, while they are given in unit of $2\mathrm{R_y}$ in this paper (see (13)). It is clear that the

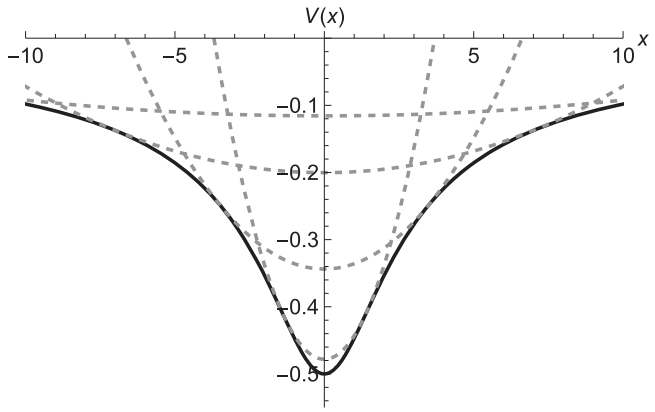

Figure 3. Four first envelopes $\tilde{V}$ (dashed gray) for $n = \{0, 1, 2, 3\}$ of the soft-Coulomb potential (solid black) for $D = 2$. All quantities are dimensionless.

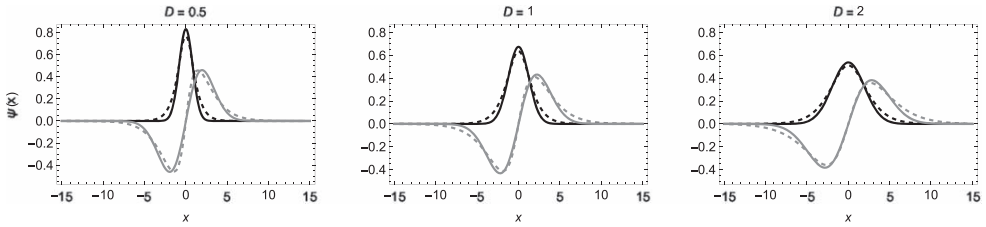

Figure 4. Ground (black) and first excited (gray) states of H for three values of D: accurate wavefunctions computed with the FGH method (dashed), and approximate wavefunctions computed with the ET (solid). All quantities are dimensionless.

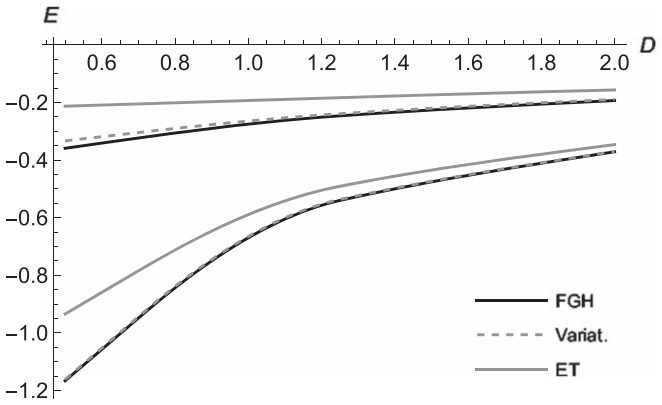

Figure 5. Dimensionless energies of the ground (3 curves below) and first excited (3 curves above) states of H as ~~un~~ function of D: accurate values obtained with the FGH method (solid black), upper bounds from the variational method in [9] (dashed gray), upper bounds from the ET (solid gray).

variational upper bounds are better that the upper bounds given by the ET. Nevertheless, the ET can give the whole spectra with a unique formula. This is not the case in [9], where different integrations must be performed to compute ground and first excited states. Moreover, the variational principle states that the expectation value of a Hamiltonian for an arbitrary trial state always gives an upper bound of the ground state. But an upper bound of an excited state can be reliably computed with a trial state if it is orthogonal to **all exact states** below this excited state [2]. So, for a one-dimensional system, an upper bound of the ground state can be computed with an even trial wave function and an upper bound of the first excited state with an odd trial wave function. The computation of the other excited states is much more complicated and requires the expansion of trial states on an (orthonormal) basis [24].

4. Conclusions

The envelope theory (ET) is useful to treat problems with a large number of particles when great accuracy is not required [25–27]. It can also be used to produce test calculations for numerical methods more accurate but more difficult to implement [28, 29]. Nevertheless, it can also be used in a pedagogical context to study solutions of time-independent Schrödinger-like equations, for the following reasons:

- The ET is very simple to implement since the solutions are obtained by solving a transcendental equation. Though the example presented here is a one-dimensional problem, the generalisation for many-body systems of identical particles in several dimensions is trivial [5].
- The eigenvalues can be computed for the whole spectrum with the same computational cost. Approximations for eigenvectors and mean values of observables are also easily computable.
- In the most favourable situations, analytical upper or lower bounds can be computed. This makes the study of quantum systems easier. Several examples are presented in [10, 13, 18].

My (CS) teaching of quantum mechanics relies mainly on [2]. Though the ET is not mentioned as a method to solve the time-independent Schrödinger equation during my lectures, I often propose to use it in projects for undergraduate students. This technique is rapidly mastered by the students to investigate various problems of quantum mechanics, for instance: the study of eigenvalues and eigenvectors for realistic Hamiltonians, comparisons of spectra between different potentials, variations of observables as a function of parameters of the Hamiltonian, properties of a system as a function of the number of particles, etc. Papers [6] and [10] have been written starting from two master thesis, while this paper comes from the third year student project of one of the authors (MB).

A lot of different problems can be examined. Here are two possible ones. The calculations performed above for the one-dimensional soft-Coulomb potential can be repeated for a lot of different interactions and/or for semirelativistic kinematics. An interesting case is the Hulthén potential on $\mathbb{R}_+$, $-k/(\exp(ax) - 1)$, which is bounded from above by $-k\exp(-ax)$ and from below by $-k/(ax)$. Analytical solutions are known for these three interactions in a one-dimensional Schrödinger equation [1]. Another problem that can be examined is the transition between a nonrelativistic regime and an ultrarelativistic one by solving for instance the semirelativistic harmonic oscillator, $H = \sqrt{p^2c^2 + m^2c^4} + kx^2$, and by examining the behaviour of the eigenvalues with m. Let us note that to solve transcendental equations based

on 3rd and 4th degree polynomials, it can be useful to consider the functions $F_{\pm}$ and $G_{\pm}$ defined in [13].

The results of the ET in dimensions greater than one can be improved by combining it with the dominantly orbital state method [6, 30]. The idea is to modify the equivalent of the quantum number Q_n appearing in these contexts. Such improvement could be possible in one dimension also by replacing $n + 1/2$ by $n + \gamma(n)$ in Q_n, in the same spirit as the modification of the WKB method proposed in [31]. The function $\gamma(n)$ could be fitted on accurate numerical results to produce better upper bounds. Similar calculations are already performed in [32].

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Data availability statement

The data that support the findings of this study are openly available at the following URL: https://notebookarchive.org/the-envelope-theory-as-a-pedagogical-tool–2023-03-97cajed/.

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