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The auxiliary field method and approximate analytical solutions of the Schrödinger equation with exponential potentials

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Abstract

The auxiliary field method is a new and efficient way to compute approximate analytical eigenenergies of the Schrödinger equation. This method has already been successfully applied to the case of central potentials of power-law and logarithmic forms. In the present work, we show that the Schrödinger equation with exponential potentials of the form $-ar^\lambda \exp(-\beta r)$ can also be analytically solved by using the auxiliary field method. Closed formulae giving the critical heights and the energy levels of these potentials are presented. Special attention is drawn to the Yukawa potential and the pure exponential potential.

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1. Introduction

Much work has been devoted to the computation of analytical solutions of the Schrödinger equation for the early years of quantum mechanics, especially when the Hamiltonian of the problem admits bound states. Indeed, it is often useful in physics to have a guess about the behavior of the eigenenergies of a system in terms of the various parameters of the Hamiltonian. This can be particularly relevant when one tries to fit the parameters of a model to some experimental data.

There are many methods allowing us to find approximate analytical solutions of the Schrödinger equation for bound state problems: the WKB method, variational method, etc (see [1] for example). Let us mention that the large- N expansion is also an interesting method [2]. In previous works [3–5], we have proposed and extensively studied a new method to compute the eigenenergies of a given Hamiltonian admitting bound states. This method is

based on auxiliary fields (also known as einbein fields [6]) and can lead to closed analytical approximate results. It has strong connections with the envelope theory [7], as shown in [8]. The general principle of the auxiliary field method (AFM) will be recalled in section 2. Up to now, the AFM has been mainly applied in the case of central potentials of the form $ar^\lambda + br^\eta$. We have shown, in particular, that the qualitative features of the exact energy spectra are well reproduced and that the analytical formulae can be greatly improved by a comparison with a numerical resolution of the problem. Then they become very accurate [3–5].

In the present work, we intend to apply the AFM to find approximate closed analytical formulae for central potentials of the exponential form, that is $-\alpha r^\lambda e^{-\beta r}$. We thus start with the following Hamiltonian:

$$H = \frac{\vec{p}^2}{2m} - \alpha r^\lambda e^{-\beta r}, \quad (1)$$

where α and β are both positive and nonzero real parameters. It is interesting to define the new variables $\{\vec{x} = \beta\vec{r}, \vec{q} = \vec{p}/\beta\}$ and to work with the dimensionless Hamiltonian $\mathcal{H} = 2mH/\beta^2$ instead of H . Indeed, one has then

$$\mathcal{H} = \vec{q}^2 - gx^\lambda e^{-x}, \quad (2)$$

with

$$g = \frac{2m\alpha}{\beta^{\lambda+2}}. \quad (3)$$

The rewriting of the problem under this particular form emphasizes the fact that the dimensionless parameter g given by (3) contains all the relevant information of H . Only the eigenenergies $\epsilon(g)$ of (2) have thus to be computed; the ‘physical’ eigenenergies will then be given by $E(m, \alpha, \beta) = \beta^2\epsilon(g)/(2m)$, a relation which expresses the scaling properties of the Schrödinger equation.

We first show in section 3 that the pure exponential potential ($\lambda = 0$) can be analytically solved using the AFM provided that the energy spectrum of the Schrödinger equation with a linearly rising potential is analytically known. The pure exponential potential is common in hadronic physics for example, when a screened confining potential is considered [9, 10]. Then, we show that some general results can be obtained for $\lambda \neq 0$ in section 4, and write an explicit energy formula for the Yukawa potential ($\lambda = -1$) in section 5. The importance of this potential in theoretical physics is such that it also deserves a specific study. By comparing our formulae to numerical results, we then show in section 6 that their accuracy for the pure exponential and the Yukawa potentials can be improved by performing some minor formal modifications.

An interesting feature of exponential potentials is that they all admit a *finite* number of bound states that depend on the dimensionless parameter g , ruling the potential depth, and defined by (3). There exists thus ‘critical heights’: potential depths beyond which new bound states appear. We refer the reader to [11] for detailed explanations about how to compute critical heights in a given potential. Accurate formulae giving these critical heights are given for the pure exponential and the Yukawa potentials. Finally, we sum up our results in section 7. The definition and the properties of the Lambert function, that will frequently appear in our calculations, are given in appendix A. Additional analytical approximations for some critical heights for the Yukawa potential are given in appendix B.

2. Auxiliary field method

2.1. General principle

We recall here the main points of the method that we presented in [3]. The problem is to find an analytical approximate solution of the eigenequation $H|\Psi\rangle = E|\Psi\rangle$, H being a Hamiltonian of the standard central form

$$H = T(\vec{p}^2) + V(r). \quad (4)$$

The procedure is the following. Let us assume that $H_A = T(\vec{p}^2) + \nu P(r)$ admits bound states with an analytical spectrum, ν being a real parameter. We thus know the solution of

$$H_A|\Psi_A(\nu)\rangle = E_A(\nu)|\Psi_A(\nu)\rangle. \quad (5)$$

Let us define the function $I(x)$ with

$$I(x) = K^{-1}(x) \quad \text{and} \quad K(x) = \frac{V'(x)}{P'(x)}, \quad (6)$$

the prime denoting the derivative with respect to x . The spectrum of the following Hamiltonian:

$$\tilde{H}(\nu) = T(\vec{p}^2) + \tilde{V}(r, \nu) \quad \text{with} \quad \tilde{V}(r, \nu) = \nu P(r) + V[I(\nu)] - \nu P[I(\nu)] \quad (7)$$

is then analytically known. Let us remark that $\tilde{V}(r, \nu)$ is of the form $C_1 P(r) + C_2$, where C_1 and C_2 are constants. These numbers are determined in order that $\tilde{V}(r)$ approximates at best the potential $V(r)$. Using (5), we have

$$E(\nu) = E_A(\nu) + V[I(\nu)] - \nu P[I(\nu)]. \quad (8)$$

The physical spectrum is finally given by the eigenstates $|\Psi_A(\nu_0)\rangle$ and the eigenenergies $E(\nu_0)$, with ν_0 such that the total energy (8) is extremal, i.e. satisfying

$$\left. \frac{\partial E(\nu)}{\partial \nu} \right|_{\nu=\nu_0} = 0. \quad (9)$$

The value of ν_0 depends on the quantum numbers of the state considered. Once ν_0 is known, the constants C_1 and C_2 can be computed. It is shown in [8] that $\tilde{V}(r_0, \nu_0) = V(r_0)$ and $\tilde{V}'(r_0, \nu_0) = V'(r_0)$, where r_0 is such that $\nu_0 = K(r_0)$.

The above method can be justified as follows. Let us assume that, instead of considering $\tilde{V}(r, \nu)$ in which ν is a constant, we consider $\tilde{V}(r, \hat{\nu})$ in which $\hat{\nu}$ is an arbitrary function. A proper elimination of this auxiliary field $\hat{\nu}$ by the following constraint $\delta_{\hat{\nu}} \tilde{V}(r, \hat{\nu})|_{\hat{\nu}=\hat{\nu}_0} = 0$ leads to the solution $\hat{\nu}_0 = K(r)$. The original Hamiltonian H (4) can then be recovered since $\tilde{V}(r, \hat{\nu}_0) = V(r)$. The essence of the AFM is then to replace this function $\hat{\nu}_0$ by the constant ν_0 . In [3], it is shown that $\nu_0 \approx \langle \Psi_A(\nu_0) | \hat{\nu} | \Psi_A(\nu_0) \rangle$. The AFM can consequently be regarded as a ‘mean field approximation’ with respect to a particular auxiliary field, which is introduced to simplify the calculations. The main technical problem is the determination of analytical solutions for (6) and (9). Such a task has already been fulfilled in a satisfactory way for many interesting and nontrivial potentials [3, 4]. As we will see in the latter, it can also be achieved for the Yukawa and the pure exponential potentials.

An estimation of the error on an exact eigenvalue E can be obtained. In [3], it is shown that

$$E(\nu_0) - E \gtrsim V(r_0) - \langle \Psi_A(\nu_0) | V(r) | \Psi_A(\nu_0) \rangle. \quad (10)$$

The rhs of this equation is the difference between the value of potential V computed at the ‘average point’ r_0 and the average of this potential for the trial state. As we are mainly interested in the computation of eigenvalues, no evaluation of the quality of the approximate eigenstate $|\Psi_A(\nu_0)\rangle$ has been performed. This will be studied in a subsequent paper.

2.2. Useful formulae

We have shown in [3] that the eigenvalues of the Hamiltonian

$$H_\eta(a) = \frac{\vec{p}^2}{2m} + a \operatorname{sgn}(\eta)r^\eta \tag{11}$$

can be written under the form

$$e_\eta(a) = \frac{2 + \eta}{2\eta} (a|\eta|)^{2/(\eta+2)} \left(\frac{N_\eta^2}{m} \right)^{\eta/(\eta+2)}, \tag{12}$$

where N_η depends on the radial n and orbital l quantum numbers, as well as on η *a priori*. An interesting feature of the AFM is that the functional form of (12) does not depend on the chosen potential $P(r)$, provided that this potential is of power-law form (typically one can choose r^2 or $-1/r$) [4]. N_η depends only on the particular form of $P(r)$: one logically obtains $N_\eta = 2n + l + 3/2$ or $n + l + 1$ according to the choice $P(r) = r^2$ or $-1/r$. Since the form of N_η is an artifact of the AFM, it can be modified to better fit the exact results. In particular, we have shown that, for any physical values of η ($\eta > -2$), a good form for N_η is given by

$$N_\eta = b(\eta)n + l + c(\eta). \tag{13}$$

Simple expressions for the functions $b(\eta)$ and $c(\eta)$ have been proposed in [3] in order to give an approximation as precise as 10^{-3} for the most interesting (the lowest) values of the quantum numbers n and l . For example,

$$b(\eta) = \frac{41\eta + 86}{13\eta + 58}, \quad c(\eta) = \frac{5\eta + 17}{2\eta + 14}, \tag{14}$$

leads to very accurate energy formulae [3]. Finally, it is worth mentioning that the energy formula (12) together with (13) and (14) gives the exact result in the following important cases:

- the harmonic oscillator, for which $N_2 = 2n + l + 3/2$;
- the Coulomb potential, for which $N_{-1} = n + l + 1$.

As we have analytical and accurate energy formulae for any power-law potential at our disposal, we will assume in this work that $P^{(\eta)}(r) = \operatorname{sgn}(\eta)r^\eta$ is a good starting point to apply the AFM. Setting $P(r) = P^{(\eta)}(r)$, we have shown in [4] that the energy spectrum of the Hamiltonian

$$H = \frac{\vec{p}^2}{2m} + V(r) \tag{15}$$

is given by

$$E(v_0) = \frac{|\eta|}{2} v_0 I(v_0)^\eta + V(I(v_0)), \tag{16}$$

the optimal value v_0 being determined from the equation

$$|\eta| v_0 I(v_0)^{\eta+2} = \frac{N_\eta^2}{m} \tag{17}$$

and the function $I(v)$ coming from the relation

$$|\eta| v I(v)^{\eta-1} = V'(I(v)). \tag{18}$$

$I(v)$ depends only on the potential $V(r)$ and not on a particular eigenstate, while v_0 depends both on the potential (through the I function) and on the state under consideration (through N_η). Equations (16)–(18) are general results of the AFM, that will be used intensively in this work.

We have shown in [4] that replacing the power η by λ does not change the functional form of $I(\nu)$ but substitutes simply the number N_η by N_λ . The AFM cannot say what is the optimal value for the power of $P(r)$. It is necessary to resort to a numerical analysis. Moreover it was also shown in [4] that the approximate eigenvalues are ruled by the correct scaling laws.

3. Pure exponential potential

3.1. Energy spectrum

The Schrödinger equation with pure exponential potential corresponds to the Hamiltonian (2) in which $\lambda = 0$, i.e.

$$\mathcal{H}_e = \vec{q}^2 - g e^{-x}. \tag{19}$$

The negative eigenenergies $\epsilon(g)$ of such a Hamiltonian can be analytically computed for $l = 0$ only. But even in this case, the expression of $\epsilon(g)$ is not very tractable since it is formally defined by relation [1]

$$J_{2\sqrt{-\epsilon(g)}}(2\sqrt{g}) = 0, \tag{20}$$

where J_ρ is a Bessel function of the first kind. Consequently, it is of interest to find an analytical energy formula for the energy levels of the pure exponential potential that is of simpler use than (20) for $l = 0$ and, above all, that remains valid for arbitrary n and l quantum numbers.

Equations (16)–(18) can be particularized in the present case. Obviously one has to set $V(x) = -g e^{-x}$ and $m = 1/2$, while a particularly convenient choice is $P(x) = P^{(1)}(x) = x$. A quick calculation leads to

$$I(\nu) = -\ln\left(\frac{\nu}{g}\right) \tag{21}$$

and to the energy formula

$$\epsilon_e(\nu_0) = -\nu_0 - \frac{\nu_0}{2} \ln\left(\frac{\nu_0}{g}\right), \tag{22}$$

where ν_0 satisfies the equation

$$-\nu_0 \left[\ln\left(\frac{\nu_0}{g}\right) \right]^3 = 2N^2. \tag{23}$$

Note that, in principle, $N = N_1$ in this last equality. But, as mentioned above, another choice N_λ with an arbitrary value of λ is *a priori* possible. It is worth noting that, from (6), we have $K(x) = g e^{-x}$ and thus $\nu_0 \in [0, g]$.

By defining

$$x_0 = \left(\frac{\nu_0}{g}\right)^{1/3} \quad \text{and} \quad Z = \frac{1}{3} \left(\frac{2N^2}{g}\right)^{1/3}, \tag{24}$$

we can recast (23) into the form

$$-x_0 \ln x_0 = Z. \tag{25}$$

$x_0 \in [0, 1]$ by definition, and the function $F(x_0) = -x_0 \ln x_0$ is such that $F(0) = F(1) = 0$, with a maximum in $F(1/e) = 1/e$. It means that (25) has no solution if $Z > 1/e$; the solution of (25) turns out to be

$$x_0(Z) = e^{W_0(-Z)} = -\frac{Z}{W_0(-Z)} \quad \text{with} \quad 0 < Z \leq 1/e, \tag{26}$$

where W_0 is the principal branch of the Lambert function, whose main properties are given in appendix A. The choice of W_0 ensures that the total energy has the correct limit for small β (see below). Equation (22) now becomes

$$\epsilon_e(v_0) = \epsilon_e(gx_0(Z)^3) = -g e^{3W_0(-Z)} \left[1 + \frac{3}{2} W_0(-Z) \right], \quad (27)$$

and the energy, rewritten in physical units, is finally given by

$$E_e = \frac{\beta^2}{2m} \epsilon_e = -\alpha e^{3W_0(-Z)} \left[1 + \frac{3}{2} W_0(-Z) \right], \quad \text{with} \quad Z = \frac{1}{3} \left(\frac{N^2 \beta^2}{m\alpha} \right)^{1/3}. \quad (28)$$

The limit $\beta \rightarrow 0$ is interesting. Indeed, $-\alpha e^{-\beta r} \approx -\alpha + \alpha\beta r$ in this case: the potential is nearly a linear confining one. Recalling that $g = 2m\alpha/\beta^2$ for the pure exponential potential, it can be checked that, at small β ,

$$E_e = -\alpha + \frac{3}{2} m^{-1/3} [\alpha\beta N]^{2/3} + O(\beta^{4/3}). \quad (29)$$

This last formula is exactly that which is expected in the case of a linear potential (see (12) for $a = \alpha\beta$ and $\eta = 1$).

For computational reasons, the Lambert function may be uneasy to deal with. We mention that we can use the approximate expression

$$e^{3W_0(-Z)} \left[1 + \frac{3}{2} W_0(-Z) \right] \approx \frac{e^{-3Z}}{100} [100 - 150Z - 580Z^2 + 524Z^3] \quad (30)$$

which leads to an absolute error below 0.008 for $0 \leq Z \leq 1/e$.

We finally point out that the energy spectrum of potentials like $(a - b e^{-cr})$ are trivially obtained by adding a constant term to formula (28). Such potentials are of interest in hadronic physics when one considers a screened confining potential to take into account possible string-breaking effects [9, 10].

3.2. Critical heights

Let us consider first the AFM framework. By definition, the critical heights g_{nl} of the exponential are such that $\epsilon_e(g = g_{nl}) = 0$, with ϵ_e given by (27). According to this last equation, one finds that the energy vanishes for $Z = 2e^{-2/3}/3$, a value which is lower than $1/e$ as required by (25). Equivalently, one can say that the critical heights are given by

$$g_{e;nl} = \frac{e^2}{4} N_{nl}^2. \quad (31)$$

They are such that, if $g > g_{n_0 l_0}$, the potential admits a bound state with the given quantum numbers n_0, l_0 . It is remarkable that our approximation scheme, based on the linear potential gx for which an infinite number of bound states are present, is able to predict that only a finite number of bound states will be present in the pure exponential potential. This is another test of the ability of the AFM to analytically reproduce the qualitative features of a given eigenvalue problem. Let us note that the AFM does not give any information about the optimal power-law potential to determine the form of the number N_{nl} .

Equation (20) can also lead to a determination of the exact (as coming from the Schrödinger equation) critical heights g_{n_0} ; let us denote them as $g_{n_0}^*$. Indeed these critical heights are such that they correspond to a energy level $\epsilon(g_{n_0}^*) = 0$. We are thus led to the equation

$$J_0(2\sqrt{g_{n_0}^*}) = 0 \Rightarrow g_{n_0}^* = \frac{J_n^2}{4}, \quad (32)$$

Table 1. Some exact critical heights $g_{e,nl}^*$ for the exponential potential $-g e^{-x}$.

n	$l = 0$	1	2	3
0	1.446	7.049	16.313	29.258
1	7.618	16.921	29.880	46.518
2	18.722	31.526	48.077	68.346
3	34.760	50.948	71.002	94.838

where j_n is the $(n + 1)$ th zero of the Bessel function J_0 . At large n , these are given by $j_n \approx \pi(n + 3/4)$ [12], leading to the asymptotic expression

$$g_{n0}^* \approx \frac{\pi^2}{4} \left(n + \frac{3}{4} \right)^2. \tag{33}$$

This result is qualitatively similar to (31), stating that $g_{n0} \propto N_{n0}^2$.

We can try to use formula (33) to improve the result (31). Assuming that $N_{nl} = bn + l + c$ with no constraint on parameters b and c (contrary to what is expected from (13)), it is easy to see that formulae (31) and (33) coincide for g_{n0} with $b = \pi/e$ and $c = 3\pi/(4e)$. We can then try a new relation to compute the critical heights

$$g_{e,nl} = \left(\frac{\pi}{2}n + \frac{e}{2}l + \frac{3\pi}{8} \right)^2. \tag{34}$$

This formula is in good agreement with exact results: for $n \in [0, 5]$ and $l \in [0, 5]$, the minimal, maximal and mean relative errors are respectively 0.03%, 8.7% and 3.5%. It is not possible to obtain so good agreement by choosing b and c values coming from (14). Some exact $g_{e,nl}^*$ values are given in table 1; they are computed numerically by solving the Schrödinger equation with a vanishing energy.

Formula (34) is fully analytical and is designed in order to reproduce correctly the behavior of the exact critical heights for large n and $l = 0$, $g_{e;n0} \approx g_{n0}^*$. Unfortunately, the analytical asymptotic expression of g_{0l}^* is not known, and an improvement of formula (34) must rely on numerical arguments, in particular using the numerical values of $g_{e,nl}^*$, as given in table 1. Moreover, a good overall fit formula needs to reproduce correctly not only the behavior in terms of n or l separately, but must try to get the good behavior in terms of n and l simultaneously. Since we want to stick as much as possible to the philosophy of AFM, we maintain the quadratic form $g_{e,nl} \propto N^2$ and just add in the expression of N a term proportional to \sqrt{nl} . Thus, we propose a new expression for the critical heights which reads

$$g_{e,nl} \approx (1.566n + 1.393l - 0.125\sqrt{nl} + 1.202)^2. \tag{35}$$

The improvement as compared to (34) is very appreciable since, in this case, the minimal, maximal and mean relative errors are respectively 0.005%, 4.5% and 1.1%.

Using (31), one can write

$$Z = \frac{2}{3} e^{-2/3} \left(\frac{g_{e,nl}}{g} \right)^{1/3}. \tag{36}$$

This makes clear the dependence on the critical heights $g_{e,nl}$ for formula (27). It is then easy to see that $\epsilon_e = 0$ when $g = g_{e,nl}$.

4. The general case

In order to compute analytically the spectrum of Hamiltonian (2) for arbitrary values of λ , it is of interest to use the general result (12), and consequently to choose $P(x) = \text{sgn}(\lambda)x^\lambda$. Equation (6) can be rewritten in the present case as

$$\hat{v} = K(x) = g \frac{e^{-x}}{|\lambda|} (x - \lambda). \tag{37}$$

The function $K(x)$ is such that $K(0) = -g \text{sgn}(\lambda)$, $K(\lambda) = 0$ and $\lim_{x \rightarrow \infty} K(x) = 0^+$. It has a maximum in $K(\lambda + 1) = g e^{-\lambda-1}/|\lambda|$, the position of this maximum being in the range $x \geq 0$ for $\lambda \geq -1$. We can conclude from this discussion that $K(x) \in [0, g]$ if $-2 < \lambda \leq -1$, $K(x) \in [0, g e^{-\lambda-1}/|\lambda|]$ if $-1 < \lambda < 0$ and $K(x) \in [-g, g e^{-\lambda-1}/|\lambda|]$ if $\lambda > 0$. In the first case, the function $K(x)$ is monotonically decreasing while in the two last cases, it presents a maximum.

The inversion of (37) can be achieved thanks to the Lambert function since $K(x)$ is of the form (A.3). One finds

$$I_\lambda(v) = \lambda - W\left(-e^\lambda |\lambda| \frac{v}{g}\right), \tag{38}$$

where one must be careful in the choice of either W_0 or W_{-1} that will depend on the particular value of λ . Nevertheless, as both branches of the Lambert function share the same properties, it is possible to go a step further in our computations by using the generic solution (38).

Let us first define

$$x_0 = \frac{|\lambda|v_0 e^\lambda}{g} \quad \text{and} \quad Y_\lambda = \frac{2N^2 e^\lambda}{g}, \tag{39}$$

where $N = N_\lambda$ *a priori*. But let us recall that another choice is possible as mentioned previously. Then, a rewriting of (16)–(18) with $V(x) = -gx^\lambda e^{-x}$, $m = 1/2$ and $P(x) = P^{(\lambda)}(x) = -\text{sgn}(x)x^\lambda$ leads to

$$\epsilon_\lambda(x_0) = -\frac{g}{2e^\lambda} x_0^{\frac{2}{\lambda+2}} Y_\lambda^{\frac{\lambda}{\lambda+2}} \left[\frac{(\lambda+2)x_0^{\frac{1}{\lambda+2}} - Y_\lambda^{\frac{1}{\lambda+2}}}{Y_\lambda^{\frac{1}{\lambda+2}} - \lambda x_0^{\frac{1}{\lambda+2}}} \right], \tag{40}$$

where x_0 is a solution of

$$x_0 [\lambda - W(-x_0)]^{\lambda+2} = Y_\lambda. \tag{41}$$

When the function $F_\lambda(x_0) = x_0 [\lambda - W(-x_0)]^{\lambda+2}$ has a maximum, it is located at

$$\bar{x}_\lambda = a_\lambda e^{-a_\lambda}, \quad \text{with} \quad a_\lambda = \frac{1}{2}(\sqrt{9+4\lambda}+3). \tag{42}$$

Note that $(3 - \sqrt{9+4\lambda})/2$ would also be a possible value for a_λ , but the choice (42) ensures that \bar{x}_λ is located in the domain of x_0 . One finds the constraint

$$Y_\lambda \leq \bar{F}_\lambda = F(\bar{x}_\lambda) = a_\lambda e^{-a_\lambda} (\lambda + a_\lambda)^{\lambda+2}. \tag{43}$$

As for the exponential potential, (40) vanishes for particular values of Y_λ , and thus critical heights appear. It can be checked that ϵ_λ is equal to zero when $Y_\lambda = 2(\lambda+2)^{\lambda+2}/e^2$, which is lower than \bar{F}_λ as demanded by (43). The critical heights are then given by

$$g_{\lambda;nl} = \left(\frac{e}{\lambda+2}\right)^{\lambda+2} N_{nl}^2. \tag{44}$$

Again, the AFM gives no information about the best form for the number N_{nl} . A first trial is to use $N = N_\lambda$ but other choices are possible. The case $\lambda = 0$ was discussed in the previous section. The case $\lambda = -1$ will be studied in the following section.

As a general result, (44) states that $g_{nl} \propto N_{nl}^2$ for any exponential potential. Interestingly, it has previously been observed that the critical heights of an arbitrary exponential potential can be very accurately fitted by a biquadratic form in n and l [13]. Our results can be seen as a demonstration of this empirical observation. However, the accuracy of the fitted form in [13] is a supplementary argument showing that the explicit form of N_{nl} cannot be computed within the AFM: only $N_{nl} = bn + l + c$ can be assumed, the coefficients b and c having to be determined by another procedure in order to improve the analytical formulae that we have obtained.

Equations (40) and (41) formally define the analytical energy formula we are looking for. Finding a general solution of (41) is a complicated problem that cannot be solved analytically. Moreover, the Yukawa potential is, to our knowledge, the only potential of common use with $\lambda \neq 0$. Before making a full treatment of the case $\lambda = -1$ in the following section, we can nevertheless make some comment about the limit where β goes to zero ($g \rightarrow \infty$ and $Y_\lambda \rightarrow 0$). In this limit, $-\alpha r^\lambda e^{-\beta r} \approx -\alpha r^\lambda$, and we should recover (12) for $\lambda < 0$ and $a = \alpha$. The nontrivial solution of (41) for $Y_\lambda = 0$ and $\lambda < 0$ is $x_0 = -\lambda e^\lambda$. It can then be checked that

$$\lim_{\beta \rightarrow 0} E_\lambda = \lim_{\beta \rightarrow 0} \frac{\beta^2}{2m} \epsilon_\lambda (-\lambda e^\lambda) = \frac{2 + \lambda}{2\lambda} (\alpha |\lambda|)^{2/(\lambda+2)} \left(\frac{N^2}{m} \right)^{\lambda/(\lambda+2)}. \quad (45)$$

This is the expected result for the energy spectrum of the potential $-\alpha/r^{|\lambda|}$. It is important to note that the trivial solution $x_0 = 0$ would lead to the unphysical limit $E_\lambda \rightarrow 0$.

In the limit $\lambda \rightarrow 0$, equation (41) reduces to

$$x_0 W(-x_0)^2 = Y_0 = (3Z)^3 \quad (46)$$

and its solution is given by

$$x_0 = -3W(-Z) e^{3W(-Z)}, \quad (47)$$

in which Z is defined by (24) (paying no attention how the number N is defined). Taking into account that $-Z \in [-1/e, 0]$, a range in which $W(-Z) < 0$, and that (40) reduces to

$$\epsilon_0 = -g x_0 \left[\sqrt{\frac{x_0}{Y_0}} - \frac{1}{2} \right], \quad (48)$$

one recovers formula (27), but with *a priori* $N = N_0$. This is an illustration that the same functional form is obtained independently of the power-law chosen for the potential $P(x)$. Moreover, $g_{\lambda=0;nl} = g_{e;nl}$ and (31) is also recovered.

Up to now, the branch to be used in these formulae is not yet determined. For $-2 < \lambda \leq -1$, the function $K(x)$ defined by (37) is monotonic and its inverse is single valued; a careful inspection of its properties shows that only the W_{-1} branch must be retained. For $\lambda > -1$, the situation is more complex and we did not find a simple prescription to fix unambiguously the type of branch. Fortunately the corresponding potentials are not of common use.

5. Yukawa potential

The Yukawa potential corresponds to the case $\lambda = -1$. A look at (37) in this case shows that one has $v_0 \in [0, g]$ and equivalently $x_0 \in [0, 1/e]$. Since $x = I_{-1}(v) \in [0, \infty[$, W_{-1} must be chosen: this branch of the Lambert function is defined on a finite domain, but can go to infinity as demanded. In this case, equations (40) and (41) read

$$\epsilon_y(\bar{Y}) = -g \frac{e x_0(\bar{Y})^2 [x_0(\bar{Y}) - \bar{Y}]}{2\bar{Y} [x_0(\bar{Y}) + \bar{Y}]}, \quad (49)$$

$$-x_0(\bar{Y})[1 + W_{-1}(-x_0(\bar{Y}))] = \bar{Y}, \quad (50)$$

where \bar{Y} denotes $Y_{-1} = 2N^2/(eg)$. Note that, in principle, $N = N_{-1}$ in this last equality. But, as mentioned above, another choice N_η with an arbitrary value of η is *a priori* possible. The function $F_{-1}(x_0) = -x_0 [1 + W_{-1}(-x_0)]$ is such that $F_{-1}(0) = F_{-1}(1/e) = 0$, with a maximum in

$$\bar{x} = \frac{3 + \sqrt{5}}{2} e^{-\frac{3+\sqrt{5}}{2}}, \quad \bar{F} = F_{-1}(\bar{x}) = (2 + \sqrt{5}) e^{-\frac{3+\sqrt{5}}{2}}. \quad (51)$$

Let us note the relation $\bar{F}/\bar{x} = \Phi = (1 + \sqrt{5})/2$, the golden ratio. Following (44), the critical heights read in this case

$$g_{y;nl} = eN_{nl}^2. \quad (52)$$

A previous formula giving analytical approximate energy levels for the Yukawa potential has been found in [14] in the framework of the envelope theory. It is given in our notations by

$$E_{nl}^{\text{up}} = \min_{x>0} \left(\frac{N_{-1}^2}{x^2} - g \frac{e^{-x}}{x} \right). \quad (53)$$

But, the result of [8] implies that E_{nl}^{up} is exactly equal to $\epsilon_y(\bar{Y})$ defined by (49) and (50). It means that the AFM and the envelope theory lead to the same approximate energy formula for the Yukawa potential, provided the quantity N is restricted to N_{-1} . Nevertheless, a closed energy formula has not been proposed in [14]; we achieve such a task in the following.

In order to have an explicit energy formula, it is of interest to find an analytical approximation for $x_0(\bar{Y})$, the solution of (50). For a given value of \bar{Y} , two values of x_0 are allowed: the first one goes to zero when \bar{Y} vanishes, and the second one tends to $1/e$ in this limit. We already mentioned that the physical solution should actually be such that $\lim_{\bar{Y} \rightarrow 0} x_0(\bar{Y}) = 1/e$ in order to find the correct Coulomb limit when $\beta \rightarrow 0$. From the study of the function $F_{-1}(x)$, it is possible to determine that $x_0(0) = 1/e$ and $x_0(\bar{F}) = \bar{x}$. Moreover, in $\bar{Y} = 0$ and $\bar{Y} = \bar{F}$, the function $x_0(\bar{Y})$ has a horizontal and a vertical tangent, respectively. So, the simplest form to parameterize $x_0(\bar{Y})$ is a branch of ellipse.

As it can be seen in figure 1, the analytical form

$$x_0(\bar{Y}, A) = \bar{x} + \left(\frac{1}{e} - \bar{x} \right) \sqrt{1 - \left(\frac{\bar{Y}}{\bar{F}} \right)^2 + A\bar{Y}(\bar{Y} - \bar{F})} \quad (54)$$

reproduces rather well the numerical solution for the simplest choice $A = 0$, but is particularly accurate for the optimal value $A = 2$. When $A \neq 0$, the curve is not a branch of ellipse and the tangent in $\bar{Y} = 0$ is not horizontal, but the global agreement is improved. Recalling that $g = 2m\alpha/\beta$ for the Yukawa potential, the final energy spectrum reads

$$E_y = \frac{\beta^2}{2m} \epsilon_y(x_0(\bar{Y}, 2)) = -\alpha\beta \frac{e^{x_0(\bar{Y}, 2)} [x_0(\bar{Y}, 2) - \bar{Y}]}{2\bar{Y} [x_0(\bar{Y}, 2) + \bar{Y}]}, \quad \text{with} \quad \bar{Y} = \frac{\beta N^2}{em\alpha}. \quad (55)$$

This formula can be recast in the following form:

$$E_y = E_{\text{Coul}} \left[e^2 x_0(\bar{Y}, 2)^2 \frac{x_0(\bar{Y}, 2) - \bar{Y}}{x_0(\bar{Y}, 2) + \bar{Y}} \right], \quad (56)$$

where E_{Coul} is the energy for a pure Coulomb potential given by

$$E_{\text{Coul}} = -\frac{\alpha^2 m}{2N^2}. \quad (57)$$

As the term within brackets in (56) tends toward 1 when $\beta \rightarrow 0$, we can expect that $N = N_{-1}$ is a good choice for small values of β . This will be examined in section 6.

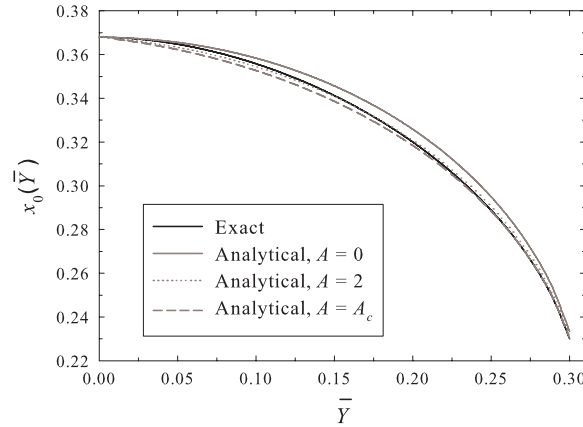


Figure 1. Plot of the exact solution of (50) (solid line), compared to the fitted form (54) with $A = 0$ (full gray line), $A = 2$ (dotted gray line) and $A = A_c \approx 2.87$ (dashed gray line). The case $A = 2$ is nearly indistinguishable from the exact solution.

Using (52), one can write

$$\bar{Y} = \frac{2}{e^2} \frac{g_{y;nl}}{g}. \tag{58}$$

This makes clear the dependence on the critical heights $g_{y;nl}$ for formulae (55) and (56). It is worth mentioning that $A = 2$ comes from a fit of formula (54) on the numerical solution of (50). Another choice could have been done, that is to set $A = A_c$ such that

$$x_0\left(\bar{Y} = \frac{2}{e^2}, A_c\right) = \frac{2}{e^2}. \tag{59}$$

Then the final energy formula exactly vanishes at the critical heights (52). One then obtains for A_c a complicated analytical formula that we do not give explicitly here; it is enough for our purpose to know that $A_c \approx 2.87$.

The results we obtained here in the most interesting case of the Yukawa potential can actually be generalized to potentials with $-2 < \lambda \leq -1$. It can indeed be numerically checked that the solution of (41) in this range is quite well fitted by the analytical form

$$x_0(Y_\lambda, A_\lambda) = \bar{x}_\lambda + (|\lambda|e^\lambda - \bar{x}_\lambda) \sqrt{1 - \left(\frac{Y_\lambda}{\bar{F}_\lambda}\right)^2 + A_\lambda Y_\lambda (Y_\lambda - \bar{F}_\lambda)}, \tag{60}$$

with

$$A_\lambda = -(109 + 196\lambda + 85\lambda^2). \tag{61}$$

This function is such that $A_{-1} = 2$. Note that the branch W_{-1} has to be chosen, by continuity with the Yukawa case in particular. Once this solution is assumed, the energy spectrum is eventually given by $\epsilon_\lambda(x_0(Y_\lambda, A_\lambda))$ (see (40) with $W = W_{-1}$).

It has been shown in [15] that the critical heights of the Yukawa potential are given with a relative accuracy around 0.4% by the following fitted form:

$$g_{nl}^G = 2 \left(\sqrt{Z_l} + \frac{n}{S_l} \right)^2, \tag{62}$$

Table 2. Some exact critical heights $g_{y,nl}^*$ for the Yukawa potential $-g e^{-x}/x$.

n	$l = 0$	1	2	3
0	1.680	9.082	21.895	40.136
1	6.447	17.745	34.420	56.514
2	14.342	29.461	49.970	75.899
3	25.372	44.261	68.572	98.318

where

$$\begin{aligned} Z_l &= Z_0(1 + \alpha l + \beta l^2), & S_l &= S_0(1 + \gamma l + \delta l^2), \\ Z_0 &= 0.839908, & \alpha &= 2.7359, & \beta &= 1.6242, \\ S_0 &= 1.1335, & \gamma &= 0.019102, & \delta &= -0.001684. \end{aligned} \tag{63}$$

Due to the smallness of γ and δ , we can replace S_l by S_0 in (62). It clearly appears that $g_{nl} \propto (S_0\sqrt{Z_0\beta}l + n)^2$ asymptotically. This quadratic behavior is predicted by our analytical results. Introducing a constant which allows us to obtain the exact result for $n = l = 0$ and considering the asymptotic expansion for large values of l , (62) is approximately given by

$$g_{nl}^G \approx (1.248n + 1.652l + 1.296)^2. \tag{64}$$

It could be interesting to improve the values of critical heights for the Yukawa potential as it was made for the pure exponential potential. Unfortunately, no analytical formula for $g_{y;n0}$ is available in this case. Nevertheless, we can assume that formula (52) is a good starting point and that $N_{nl} = bn + l + c$ with no constraint on parameters b and c (contrary to what is expected from (13)). If the two exact values $g_{y;00}^*$ and $g_{y;10}^*$ are known, the choice $b = \sqrt{g_{y;10}^*/e} - \sqrt{g_{y;00}^*/e}$ and $c = \sqrt{g_{y;00}^*/e}$ insures that (52) gives the correct critical heights for $l = 0$ and $n = 0$ and 1. Instead of using exact numerically computed values, we can use analytical approximate evaluations of these quantities (see appendix B). We can then try a new relation to compute the critical heights

$$g_{y;nl} = ([\sqrt{g_{y;10}} - \sqrt{g_{y;00}}]n + \sqrt{el} + \sqrt{g_{y;00}})^2. \tag{65}$$

With the exact critical heights, we have

$$g_{y;nl} \approx (1.243n + 1.649l + 1.296)^2, \tag{66}$$

while with the use of approximations (B.2), we have

$$g_{y;nl} \approx (1.291n + 1.649l + 1.296)^2. \tag{67}$$

These formulae are in good agreement with (64) and with exact results: for $n \in [0, 4]$ and $l \in [0, 4]$, the minimal, maximal and mean relative errors are respectively 0.005%, 4.5% and 1.2% with (66) and respectively 0.04%, 5.8% and 3.4% with (67). It is not possible to obtain so good agreement by choosing b and c values coming from (14). Let us note that the minimal, maximal and mean relative errors are respectively 0.01%, 0.9% and 0.3% with formula (62). The very good quality of these results is due to the use of a complicated formula fitted on exact results. Our formulae are simpler and the general behavior is predicted by the AFM. Some exact $g_{y,nl}^*$ values are given in table 2; they are computed numerically by solving the Schrödinger equation with a vanishing energy.

In the very same way that we improved the critical heights of the pure exponential potential, it is possible to improve the corresponding Yukawa quantities with the same kind of prescription. Here we propose the expression

$$g_{y;nl} \approx (1.247n + 1.680l - 0.054\sqrt{nl} + 1.296)^2. \tag{68}$$

In this case, the minimal, maximal and mean relative errors are respectively 0.002%, 2.4% and 0.6%. We obtain a quality of the same order than that obtained with formula (62), but with a much simpler expression.

6. Improved energy formulae

In the previous sections, approximate analytical forms for solutions of a pure exponential or a Yukawa potentials were found. The formulae depend on the quantum numbers n and l through a factor N . This number could be taken as N_λ without information about the optimal value for λ . If we look for instance at the Yukawa potential, it is clear that it reduces to a pure Coulomb interaction when $\beta = 0$. In this case, the choice $N = N_{-1}$ gives the exact result in this limit.

The dimensionless Hamiltonians considered above depend on a parameter g . The variation of the eigenvalues being smooth for the variation of g , we can assume that the number N , giving the optimal values for all the eigenvalues of a Hamiltonian, is also a smooth function of g . From considerations above, the functional form

$$N(g) = b(g)n + l + c(g) \quad (69)$$

seems reasonable. As we cannot predict the correct behavior, it is necessary to focus our attention on numerical solutions.

Very accurate eigenvalues $\epsilon_{\text{num}}(g; n, \ell)$ for Hamiltonians defined above can be obtained numerically with the Lagrange mesh method [16]. It is very accurate and easy to implement. In order to find the best possible values for coefficients $d(g)$ (d stands for b or c), we will use the following measure:

$$\chi(g) = \sum_{\{n,l\}} (\epsilon_{\text{num}}(g; n, \ell) - \epsilon_{\text{app}}(g; n, \ell))^2, \quad (70)$$

where $\epsilon_{\text{app}}(g; n, \ell)$ are values obtained from our approximate formulae. Other choices are possible but we find this one very convenient. The summation in (70) runs *a priori* on all possible pairs $\{n, l\}$ for the bound states allowed by the value of g . But for some special pairs $\{n, l\}$, the value $\epsilon_{\text{app}}(g; n, \ell)$ can be a complex number (condition (41) is not fulfilled) or a positive number (quality of approximation is poor). This drawback can happen for the highest levels. In this case, the pair $\{n, l\}$ is not taken into account in (70).

The analytical form ϵ_{app} depends on $N(g)$, which depends on coefficients d . For each value of g , optimal values for the d coefficients, $d_{\text{min}}(g)$, can be determined by minimizing $\chi(g)$. Then, with a set $\{d_{\text{min}}(g)\}$ for a given set $\{g\}$, a functional form $d_{\text{fit}}(g)$ can be fitted with the following measure (χ' is also a chi-square fit, but the prime indicates that the function χ' is indeed different from χ in (70)):

$$\chi'(d) = \sum_{\{g\}} (d_{\text{min}}(g) - d_{\text{fit}}(g))^2. \quad (71)$$

Again, other choices are possible but we find this one very convenient. We will now try to determine the best form of coefficients $d(g)$ for the potentials studied above.

6.1. Pure exponential potential

Approximate dimensionless eigenvalues for the pure exponential potential are given by (27). By minimizing our measure $\chi(g)$, we found the optimal values of $b(g)$ and $c(g)$ for several finite values of g . We tried to fit these numerical points with various functions and found that the

Table 3. Quality of formula (27) with parameterization (72) for a pure exponential potential.

g	5	10	20	40	60	80	100
R	1/1	3/3	4/6	7/10	12/15	15/20	19/26
$\Delta_{\min.}$	0.8	4.1	1.7	1.6	0.4	0.5	0.3
$\Delta_{\max.}$	0.8	54.6	79.7	35.0	98.5	91.2	81.7
Δ_{mean}	0.8	31.6	22.6	11.8	23.6	18.3	19.1

R : (number of negative eigenvalues found)/(total number of bound states).

$\Delta_{\min./\max.}$: minimal/maximal relative error (%) for negative eigenvalues found.

Δ_{mean} : mean relative error (%) computed with all negative eigenvalues found.

Table 4. Eigenvalues for a pure exponential potential with $g = 40$ as a function of $\{l, n\}$ sets.

l	$n = 0$	1	2	3
0	-17.53	-6.88	-1.87	-0.077
	-17.84	-7.58	-1.59	*
1	-10.14	-3.35	-0.42	-
	-9.98	-2.99	*	-
2	-5.03	-0.93	-	-
	-4.63	*	-	-
3	-1.55	-	-	-
	-1.01	-	-	-

* Indicates a non-real or a non-negative value.

First line: exact value.

Second line: formula (27) with parameterization (72).

best result is obtained for sections of hyperbola, for both $b(g)$ and $c(g)$. The parameterization retained is

$$b(g) = \frac{1.42g - 12.76}{g - 8.62}, \quad c(g) = \frac{1.32g + 16.88}{g + 14.95}. \quad (72)$$

The quality of this parameterization for both $b(g)$ and $c(g)$ in (27) can be appraised in tables 3 and 4. Not all bound states can be found. As in (70), only real strictly negative eigenvalues are retained. The mean relative error is about 20% but the accuracy is much better for the lowest eigenvalues.

When $\beta \rightarrow 0$, that is $g \rightarrow \infty$, the pure exponential potential reduces at first order to a constant and at the next order to a linear potential. Relations (72) show that $\lim_{g \rightarrow \infty} b(g) = 1.42$ and that $\lim_{g \rightarrow \infty} c(g) = 1.32$. These numbers are different from the values $b \approx 1.79$ and $c \approx 1.38$ expected for a linear potential, and from $b \approx 1.48$ and $c \approx 1.21$ expected for constant potential (see (14)). We will see that the situation will be clearer for the Yukawa potential.

6.2. Yukawa potential

Approximate dimensionless eigenvalues for the Yukawa potential are given by (49) supplemented by (54). In all results presented, we chose $A = 2$. By using a similar procedure as those described for the pure exponential potential, we found that the best result

Table 5. Quality of various approximations for the Yukawa potential.

g	5	10	20	30	40	50
R	1/1	2/3	3/5	6/8	6/10	10/13
	1/1	1/3	3/5	6/8	6/10	10/13
	1/1	3/3	5/5	8/8	10/10	12/13
$\Delta_{\min.}$	0.2	0.07	0.0006	0.02	0.02	0.02
	13.5	3.5	1.3	0.8	0.6	0.5
	0.4	0.1	0.06	0.04	0.03	0.02
$\Delta_{\max.}$	0.2	4.3	6.6	27.8	9.4	42.4
	13.5	3.5	14.1	45.6	19.2	57.3
	0.4	10.9	14.0	34.9	575.2 ^a	24.6
Δ_{mean}	0.2	2.2	3.2	13.0	4.6	16.2
	13.5	3.5	7.7	19.6	8.2	21.2
	0.4	6.4	3.3	9.8	59.5 ^a	3.9

^a The abnormally large values are due to the existence of a nearly zero eigenvalue which is badly reproduced.

R : (number of negative eigenvalues found)/(total number of bound states).

$\Delta_{\min./\max.}$: minimal/maximal relative error (%) for negative eigenvalues found.

Δ_{mean} : mean relative error (%) computed with all negative eigenvalues found.

First line: formulae (49) and (54) with parameterization (73).

Second line: formulae (49) and (54) with $N = N_{-1}$.

Third line: formula (74).

in fitting the numerical points is obtained for sections of hyperbola, for both $b(g)$ and $c(g)$. The parameterization retained is

$$b(g) = \frac{1.00g - 5.92}{g - 5.08}, \quad c(g) = \frac{1.00g - 1.68}{g - 1.58}. \quad (73)$$

As expected, $N(g) \rightarrow N_{-1}$ when $g \rightarrow \infty$, that is to say when $\beta \rightarrow 0$, since in this limit the Yukawa potential tends toward a pure Coulomb interaction. So, in the following, we will also consider the choice $N = N_{-1}$, that is $b = c = 1$.

An accurate energy formula has been found in [15] from a fit of the numerically computed energy levels of the Yukawa potential. In our notations, it reads

$$\epsilon_{nl} = -\frac{g}{4N_{nl}^2} (g - g_{nl}^G) \frac{g - 2A'(N_{nl} + \sigma)^2 + 2B'N_{nl}^2}{g - g_{nl}^G + 2B'N_{nl}^2}, \quad (74)$$

where $A' = 1.9875$, $B' = 1.2464$ and $\sigma = 0.003951$, where $N_{nl} = n + l + 1$ as in the Coulomb case, and where g_{nl}^G is defined by (62). This formula is rather different from ours, given by (49). However, they coincide at the limit $g \rightarrow \infty$.

The quality of the various approximations can be appraised in tables 5 and 6. Not all bound states can be found, even if formula (74) gives generally the correct number of bound states. As in (70), only real strictly negative eigenvalues are retained. Formula (49) with approximation (54) and parameterization (73) gives quite good results. The mean relative error is about 10% but the accuracy is much better for the lowest eigenvalues. The quality of the fit for formula (74) and our approach is in average quite comparable. But formula (74) is empirical. Conversely, (49) is obtained from an explicit analytical resolution of the Schrödinger equation. Our results are not so good by choosing the parameterization $N = N_{-1}$ but the quality is still reasonable.

Table 6. Eigenvalues for a Yukawa potential with $g = 30$ as a function of $\{l, n\}$ sets.

l	$n = 0$	1	2	3
0	-196.44	-31.51	-5.47	-0.22
	-196.41	-32.31	-4.16	*
	-194.82	-29.66	-2.97	*
	-196.36	-31.62	-5.67	-0.30
1	-30.74	-4.94	-0.029	-
	-29.84	-3.57	*	-
	-29.66	-2.97	*	-
	-30.52	-4.85	-0.019	-
2	-3.81	-	-	-
	-3.02	-	-	-
	-2.97	-	-	-
	-3.70	-	-	-

* Indicates a non-real or a non-negative value.

First line: exact value.

Second line: formulae (49) and (54) with parameterization (73).

Third line: formulae (49) and (54) with $N = N_{-1}$.

Fourth line: formula (74).

7. Summary of the results

The AFM was proposed in [3–5] as a tool to compute approximate analytical solutions of the Schrödinger equation. The basic idea underlying this method is to replace an arbitrary potential $V(r)$, for which no analytical spectrum is known, by an expression of the type $\tilde{V}(r) = \nu P(r) + g(\nu)$, $P(r)$ being a potential for which analytical eigenenergies can be found, ν a number (the auxiliary field) and $g(\nu)$ a well-defined function of this extra parameter. The auxiliary field is eventually eliminated by a condition rendering the eigenenergies extremal. The optimal value of ν is such that $\tilde{V}(r)$ is close to $V(r)$. Analytical closed approximate solutions can be found in favorable cases, and it is shown in [3–5] that this method is a kind of mean field approximation.

In the present work, we have searched for closed solutions of the Schrödinger equation with exponential potential of the form $-\alpha r^\lambda e^{-\beta r}$ using the AFM. Such potentials are of great interest in various fields of physics. General analytical results have been obtained for the eigenvalues of this type of potentials. It is proved that the critical heights for these interactions are proportional, with a good approximation, to $(bn + l + c)^2$ where b and c are constant parameters.

We have focused our attention on pure exponential and Yukawa interactions. Approximate analytical formulae have been found for these two particular cases for arbitrary values of n and l . Some results were previously obtained for the Yukawa potential [14, 17] but, up to our knowledge, it is the first time that a closed energy formula is computed from the Schrödinger equation. The majority of eigenvalues can be computed, with a quite good accuracy, mainly for lowest states. In particular, it is shown that this accuracy can be improved by slight modifications given by a comparison with exact results coming from a numerical analysis. Moreover, very simple analytical approximate formulae have been obtained for the critical heights of these two potentials.

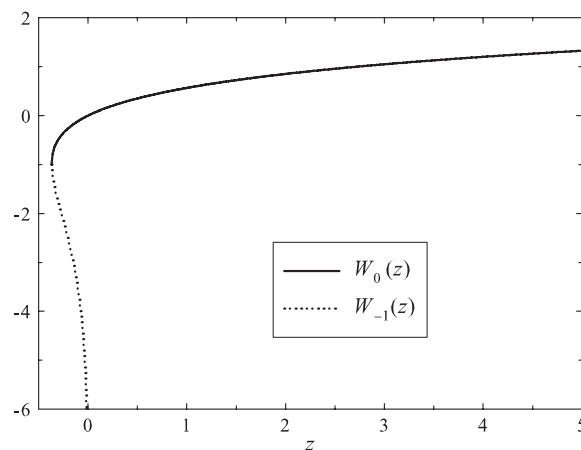


Figure A1. Plot of the two branches of the Lambert function, namely $W_0(z)$ (solid line) and $W_{-1}(z)$ (dotted line).

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Appendix A. The Lambert function

Let us briefly recall some points concerning the Lambert function (also called Omega function or product-log) that we will denote $W(z)$. First, $W(z)$ is defined as the inverse function of $z e^z$. Consequently, it has the following properties:

$$W(z) e^{W(z)} = W(z e^z) = z, \tag{A.1}$$

$$\partial_z W(z) = \frac{W(z)}{z[1 + W(z)]}. \tag{A.2}$$

But, it is readily observed that the inverse function of $z e^z$ is multivalued. Two branches of the Lambert function thus exist, respectively denoted as $W_0(z)$, defined for $z \geq -1/e$, and $W_{-1}(z)$, defined for $-1/e \leq z \leq 0^3$. They are plotted in figure A1. Obviously, both branches of the Lambert function share the same properties (A.1) and (A.2) as $W(z)$; they meet in $W_{-1}(-1/e) = W_0(-1/e) = -1$. It can moreover be checked that $W_0(|x| \ll 1) \approx x$, $\lim_{x \rightarrow 0} W_{-1}(x) = -\infty$ and $\lim_{x \rightarrow \infty} W_0(x) = \infty$.

For our purpose, it is worth mentioning that the equation

$$(az + b)^n e^{-z} = \theta \tag{A.3}$$

is analytically solvable with the Lambert function. One has

$$z = -\frac{b}{a} - nW \left[-\frac{1}{an} (e^{-b/a}\theta)^{1/n} \right], \tag{A.4}$$

where either W_0 or W_{-1} has to be chosen following the range of θ and z that the function $z(\theta)$ has to cover.

³ Note that the two branches $W_0(x)$ and $W_{-1}(x)$ of the Lambert function $W(x)$ are known by the software *Mathematica* package as `ProductLog[0, x]` and `ProductLog[-1, x]`, respectively.

Appendix B. Analytical estimation of critical heights g_{n0} for the Yukawa potential

In [18], it is shown that, for a fixed value of the parameter a , solutions of the equation

$$\frac{d^2\phi}{dx^2} + \left(a + b\frac{e^{-x}}{x}\right)\phi = 0, \quad (\text{B.1})$$

with the boundary conditions $\phi(0) = \phi(\infty) = 0$, can be accurately obtained by a variational method. The eigenvalues b are given by the extremum of the ratio J/N , where the quantities J and N are, respectively, given by equations (18) and (19) in [18] (note a misprint: parameter b must not be present in (19)). This ratio J/N depends on a and on $n + 1$ linear variational parameters h_v . The critical heights g_{n0} we search for are given by $\lim_{a \rightarrow 0} b$.

For $n = 0$, the only solution, which is independent of h_0 (normalization condition), is given by $g_{00} = 1/\ln(16/9) \approx 1.738$. This value is not too far from the exact one (see table 2). For $n = 1$, two extrema for J/N exist and depend on h_1/h_0 . They can be obtained analytically, but their expressions are very complicated and unusable in practice. Nevertheless, the two optimal values for h_1/h_0 are very close to -2 and $1/2$, respectively. So we can set

$$\begin{aligned} g_{00} &\approx \frac{J}{N} \Big|_{h_1/h_0=1/2} = \frac{17}{6 \ln(27/5)} \approx 1.680, \\ g_{10} &\approx \frac{J}{N} \Big|_{h_1/h_0=-2} = \frac{1}{60 \ln(2) - 26 \ln(3) - 8 \ln(5)} \approx 6.693. \end{aligned} \quad (\text{B.2})$$

These two values are good approximations of the exact ones.

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