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# Energy-dependent potentials and the problem of the equivalent local potential

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## Abstract

The properties of the wave equation are studied in the case of energy-dependent potentials for bound states. The nonlinearity induced by the energy dependence requires modification of the standard rules of quantum mechanics. These modifications are briefly recalled. Analytical and numerical solutions are given in the three-dimensional space for power-law radial shape potentials with a linear energy dependence. This last is chosen since it allows the construction of a coherent theory. Among the results, we stress the saturation of the spectrum observed for confining potentials: as the quantum numbers increase, the eigenvalues reach an upper limit. Finally, the problem of the equivalent local potential is discussed. The existence of analytical solutions presents a good opportunity to tackle this problem in detail.

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(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

Wave equations with energy-dependent potentials have been known in physics for a long time. They occur in relativistic quantum mechanics, first with the Pauli–Schrödinger equation [1]. Recently, they appear in the Hamiltonian formulation of the relativistic many-body problem in connection with the manifestly covariant formalism with constraints [2–4]. They also play a role in non-relativistic physics offering the possibility of studying nonlinear effects in the framework of the Schrödinger equation. Energy-dependent potentials have been used as a source of nonlinear Hamiltonian evolution equations [5–8]. They are currently applied to soliton propagation [9–11]. However, to our knowledge, the case for bound states has retained little attention.

In a recent paper, the properties of the wave equations with an energy-dependent potential were investigated, together with the necessary conditions to be imposed for such a theory to

be coherent [12]. This paper gives the solutions for the harmonic oscillator in one dimension. Extensions to the three-dimensional space were presented in [13], in connection with the heavy charmonia and bottomia spectra.

The present work is devoted to potentials with power-law radial shapes in the three-dimensional space, for which analytical solutions exist in few cases. The energy dependence is chosen to be linear. In fact, the energy dependence is not given by general principles. It should be derived from the underlying theory. Thus, fixing the energy dependence *a priori* is arbitrary. The choice of a linear dependence is motivated by the fact that in this case it can be shown to lead us to a coherent theory [12].

The study of power-law potentials offers the possibility of dealing with the question of the local equivalent potential. It has been shown by Formanek *et al* [12] that in the case of a linear dependence, the problem can be reformulated as an ordinary Schrödinger equation with a non-local potential<sup>3</sup>. The existence of analytical solutions provides a good opportunity to investigate the question of the local equivalent potential. As far as we know, this problem has not yet been discussed in detail in the case of bound states.

The paper is organized as follows. In section 2, we shall recall the basic aspects of the wave equation with energy-dependent potentials. Solutions will be given for power-law potentials in section 3, together with a study of the saturation effect: for potentials with a confining radial shape, the eigenvalues reach an upper limit as the quantum numbers increase. The question of equivalent local potential is the subject of section 4. Conclusions are drawn in section 5.

## 2. The wave equation

The presence of an energy-dependent contribution in the potential has several implications modifying the usual rules of quantum mechanics. They reflect the nonlinearity of the problem and are necessary to establish a coherent theory. Most of them are well known. Derivations can be found in previous works.

Many authors have noted that the density probability, or the scalar product, has to be modified with respect to the usual definition, in order to satisfy the continuity equation [14, 15]. It is easy to show that the continuity equation is satisfied if the density is defined by

$$\rho(\vec{r}, t) = \Psi^*(\vec{r}, t) \left[ 1 - \frac{V(\vec{r}, E') - V(\vec{r}, E)}{E' - E} \right] \Phi(\vec{r}, t). \quad (1)$$

Accordingly, the scalar product is written as

$$\langle \Psi | \Phi \rangle = \int \Psi^*(\vec{r}) \left[ 1 - \frac{V(\vec{r}, E') - V(\vec{r}, E)}{E' - E} \right] \Phi(\vec{r}) d\vec{r}. \quad (2)$$

The use of  $\langle \cdot | \cdot \rangle$  is made here to distinguish the new scalar product from the usual form  $\langle \cdot | \cdot \rangle$ . As  $E' \rightarrow E$ , the wavefunction  $\Phi(\vec{r}) \rightarrow \Psi(\vec{r})$ , and the norm is given by

$$\langle \Psi | \Psi \rangle = \int \Psi^*(\vec{r}) \left[ 1 - \frac{\partial V(\vec{r}, E)}{\partial E} \right] \Psi(\vec{r}) d\vec{r}. \quad (3)$$

We note that for  $\rho(\vec{r}) = \Psi^*(\vec{r})\Psi(\vec{r})$  to represent a density, it has to be positive definite. This is ensured if and only if

$$\left[ 1 - \frac{\partial V(\vec{r}, E)}{\partial E} \right] > 0. \quad (4)$$

<sup>3</sup> Strictly speaking, a non-local potential depends on two space variables. For the sake of simplifying the language,  $V(\vec{r}, \vec{p})$  and  $V(\vec{r}, E)$  will be quoted as non-local potentials on the ground that they depend on momentum or energy besides a single space variable.

Consider two eigenfunctions  $\Psi_i(\vec{r})$  and  $\Psi_j(\vec{r})$  with the eigenvalues  $E_i$  and  $E_j$ , respectively. The orthonormality relation is written as

$$\langle \Psi_i | \Psi_j \rangle = \int \Psi_i^*(\vec{r}) [1 - \varphi_{ij}(\vec{r})] \Psi_j(\vec{r}) d\vec{r} = \delta_{ij}, \tag{5}$$

with

$$\varphi_{ij}(\vec{r}) = \frac{V(\vec{r}, E_i) - V(\vec{r}, E_j)}{E_i - E_j} \quad i \neq j, \tag{6}$$

and

$$\varphi_{ii}(\vec{r}) = \frac{\partial V(\vec{r}, E)}{\partial E}. \tag{7}$$

As stated in the introduction, the energy dependence is not dictated by general principles but it should be derived from the underlying theory. On the other hand, a linear dependence has interesting properties: it produces a coherent theory, and it can be reformulated as an ordinary quantum mechanics with a non-local potential [12].

To illustrate the particularity of the linear energy dependence, we can look at one of the consequences of the closure relation. Consider the function

$$\Psi(\vec{r}) = \sum_i c_i \Psi_i(\vec{r}). \tag{8}$$

We have obviously

$$c_i = \int \Psi_i^*(\vec{r}') [1 - \varphi_{ii}(\vec{r}')] \Psi(\vec{r}') d\vec{r}'. \tag{9}$$

Inserting (9) in (8) and inverting the sum and the integral yields

$$\Psi(\vec{r}) = \int d\vec{r}' \Psi(\vec{r}') \sum_i \Psi_i^*(\vec{r}') [1 - \varphi_{ii}(\vec{r}')] \Psi_i(\vec{r}). \tag{10}$$

This equation is satisfied if we consider

$$\sum_i \Psi_i^*(\vec{r}') [1 - \varphi_{ii}(\vec{r}')] \Psi_i(\vec{r}) = \delta(\vec{r} - \vec{r}'). \tag{11}$$

Suppose that (11) is actually a delta-function; then

$$\begin{aligned} \Psi_j(\vec{r}) &= \int \Psi_j(\vec{r}') \sum_i \Psi_i(\vec{r}') [1 - \varphi_{ii}(\vec{r}')] \Psi_i^*(\vec{r}) d\vec{r}' \\ &= \sum_i \int \Psi_j(\vec{r}') [1 - \varphi_{ij}(\vec{r}') - (\varphi_{ii}(\vec{r}') - \varphi_{ij}(\vec{r}'))] \Psi_i^*(\vec{r}') d\vec{r}' \\ &= \Psi_j(\vec{r}) - \sum_i \Psi_i(\vec{r}) \int \Psi_j(\vec{r}') [\varphi_{ii}(\vec{r}') - \varphi_{ij}(\vec{r}')] \Psi_i^*(\vec{r}') d\vec{r}'. \end{aligned} \tag{12}$$

The equality is satisfied if the  $\varphi_{ij}$  are independent of the state, which is obviously the case for a linear energy dependence.

### 3. The power-law potentials

To get an insight into the way the Schrödinger equation is handled in the case of energy-dependent potentials, we study in this section the solutions of a few examples with radial shapes corresponding to power-law potentials:

$$V(r) = \text{sign}(\alpha) \lambda r^\alpha.$$

Here,  $\lambda$  is the strength (coupling) constant. Spherical symmetry is assumed.

Consider the wave equation in the three-dimensional space ( $\hbar = m = 1$ ):

$$\left[-\frac{1}{2}\Delta + V_0(r) + EV_1(r)\right] \Psi(\vec{r}) = E\Psi(\vec{r}). \tag{13}$$

The linear momentum is given by [12, 16]

$$\vec{P} = -i\vec{\nabla} + i\frac{\vec{\nabla}V_1(r)}{2[1 - V_1(r)]}. \tag{14}$$

In the case of spherical symmetry, the second contribution is proportional to  $\vec{r}$ . Thus, it does not contribute to the vectorial product  $\vec{r} \times \vec{P}$ , and the angular momentum operator  $\vec{L}$  takes its usual expression.

Under spherical symmetry, the usual variable separation leads to

$$\Psi_{n\ell m}(\vec{r}) = \frac{\Phi_{n\ell}(r)}{r} Y_{\ell m}(\theta, \varphi). \tag{15}$$

Here,  $Y_{\ell m}(\theta, \varphi)$  are the spherical harmonics. The remaining equation to be solved reads

$$-\frac{1}{2}\Phi_{n\ell}''(r) + \left[\frac{\ell(\ell+1)}{2r^2} + V(r, E_{n\ell})\right] \Phi_{n\ell}(r) = E_{n\ell}\Phi_{n\ell}(r). \tag{16}$$

The searched solutions are subject to the usual boundary conditions, namely  $\Phi_{n\ell}(0) = \Phi_{n\ell}(\infty) = 0$ , together with the square integrability of  $\Psi_{n\ell m}(\vec{r})$ . The potentials we consider are of the form

$$V(r, E) = V_0(r)(1 + \gamma E). \tag{17}$$

The positivity of the density imposes

$$1 - \gamma V_0(r) > 0. \tag{18}$$

Note that for these potentials, it is the coupling constant which is energy dependent. Thus, if  $V_0(r)$  admits analytical solutions, the solutions have the same analytical expressions in the energy-dependent case. The difference is that the basic parameter appearing in the eigenvalues is linked to the coupling constant through an energy-dependent relation. Consequently, the eigenvalue equations are no longer linear, but of higher order. In this respect, it is very important to verify that a single root is attached to each state. The other roots are rejected on the ground of the square integrability of the wavefunctions.

As far as potentials admitting analytical solutions are concerned three examples are sketched.

### 3.1. $\alpha = -1$ (Coulomb)

This potential is given by

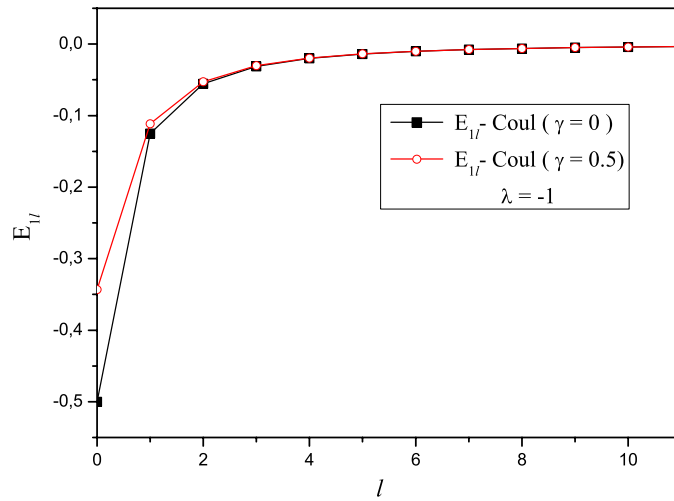
$$V(r, E_{n\ell}) = \frac{\lambda}{r}(1 + \gamma E_{n\ell}), \quad \text{with } \lambda < 0. \tag{19}$$

The potential being negative, condition (18) requires  $\gamma > 0$ . The reduced radial wavefunctions take the usual form

$$\Phi_{n\ell}(r) = C_{n\ell} r^{\ell+1} e^{-a_{n\ell}r/2} P_{n\ell}(r), \tag{20}$$

with  $P_{n\ell}(r)$  being the polynomial form of the confluent hyper-geometric functions. As can be verified, the quantization condition implies

$$a_{n\ell} = -2\lambda \frac{1 + \gamma E_{n\ell}}{n + \ell}, \quad n = 1, 2, 3, \dots, \tag{21}$$



**Figure 1.** Behavior of the spectrum of the Coulomb potential  $V(r, E)$  for  $\gamma = 0.5$  compared to ( $\gamma = 0$ ) for  $\lambda = -1$ .

while we have

$$E_{n\ell} = -\frac{1}{8}a_{n\ell}^2. \tag{22}$$

Consequently, the eigenvalues are the solutions of a second-order equation with two roots

$$E_{n\ell}^{\pm} = \frac{1}{\lambda^2\gamma^2}[-(n + \ell)^2 - \gamma\lambda^2 \pm (n + \ell)\sqrt{(n + \ell)^2 + 2\gamma\lambda^2}]. \tag{23}$$

It is easy to show that  $E_{n\ell}^-$  leads to the negative values of  $a_{n\ell}$ , which is unacceptable. Thus, only  $E_{n\ell}^+$  are retained. From now on we shall omit to specify the + exponent.

The eigenvalues  $E_{1\ell}$  are displayed in figure 1 up to  $\ell = 10$ , for  $\lambda = -1$ ,  $\gamma = 0$  and  $\gamma = 0.5$ . It shows the energy dependence to affect essentially the lowest levels. Indeed, in the limit of large quantum numbers, we get

$$\lim_{n\ell \rightarrow \infty} E_{n\ell} \approx -\frac{\lambda^2}{2(n + \ell)^2}, \tag{24}$$

which is the usual expression.

### 3.2. $\alpha = 2$ (harmonic oscillator)

Here, we have

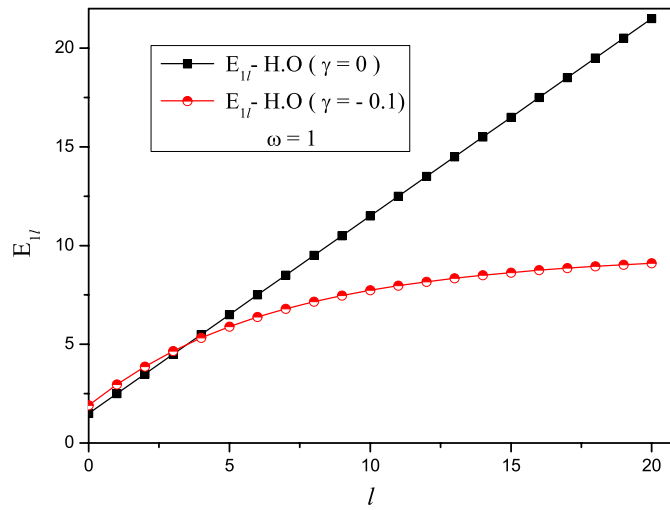
$$V(r, E_{n\ell}) = \lambda r^2(1 + \gamma E_{n\ell}). \tag{25}$$

Since  $\lambda > 0$ , the positivity of the density requires  $\gamma \leq 0$ . The reduced radial wavefunctions take the form

$$\Phi_{n\ell}(r) = C_{n\ell}r^{\ell+1}e^{-a_{n\ell}r^2/2}P_{n\ell}(r). \tag{26}$$

As for the preceding example, two conditions link the eigenvalues and  $a_{n\ell}$ :

$$\frac{2\ell - 1}{4} - \frac{E_{n\ell}}{2a_{n\ell}} = -n \quad \text{with } n = 1, 2, 3 \dots \tag{27}$$



**Figure 2.** Behavior of the spectrum of the harmonic oscillator potential  $V(r, E)$  for  $\gamma = -0.1$  compared to ( $\gamma = 0$ ) for  $\lambda = 0.5$ .

and

$$E_{n\ell} = \frac{a_{n\ell}}{2}(4n + 2\ell - 1). \tag{28}$$

As a result, the eigenvalues are the roots of a second-order equation:

$$E_{n\ell}^{\pm} = \frac{\gamma\lambda}{4}(4n + 2\ell - 1)^2 \pm \frac{4n + 2\ell - 1}{4} \sqrt{[\gamma\lambda(4n + 2\ell - 1)]^2 + 8\lambda}. \tag{29}$$

Recalling that  $\lambda > 0$  and  $\gamma \leq 0$ , only  $E_{n\ell}^+$  is positive definite together with its corresponding  $a_{n\ell}$ . The other root leads to the negative values of  $a_{n\ell}$  and thus is to be rejected. The + exponent will be omitted in what follows.

The interesting feature of the spectrum is the saturation effect, already mentioned by Formanek *et al* for the ( $D = 1$ )-dimensional case. As the quantum numbers increase, the eigenvalues reach an upper limit. From  $E_{n\ell}$  of (29), it is easy to show that

$$\lim_{n\ell \rightarrow \infty} E_{n\ell} = \frac{1}{|\gamma|}. \tag{30}$$

An illustrative example is displayed in figure 2, where the spectrum of the  $\{1\ell\}$  states is plotted up to  $\ell = 20$  for  $\lambda = 0.5$ ,  $\gamma = 0$  and  $-0.1$ .

### 3.3. $\alpha = 1$ (linear potential)

This potential is given by

$$V(r, E_{n\ell}) = \lambda(1 + \gamma E_{n\ell})r, \quad \lambda > 0. \tag{31}$$

As for all confining potentials, the condition on the density imposes  $\gamma < 0$ . For the  $\ell = 0$  states, the linear potential has analytical solutions which are well known. For the sake of clarity, we recall that introducing

$$2\lambda(1 + \gamma E_{ns}) = \frac{1}{\rho_{ns}^3}, \quad 2E_{ns} = \frac{\delta_{ns}}{\rho_{ns}^2}, \tag{32}$$

together with the change of variable

$$z = \frac{r}{\rho_{ns}} - \delta_{ns} \tag{33}$$

transforms the radial Schrödinger equation into the Airy differential equation

$$\Phi''_{ns}(z) - z\Phi_{ns}(z) = 0. \tag{34}$$

It is solved with  $\Phi_{ns}(-\delta_{ns}) = \Phi_{ns}(\infty) = 0$  as boundary conditions. The solutions are expressed by the Airy function  $\mathcal{Ai}(z)$  [17]. The zeros of the Airy function are tabulated, and the boundary condition at  $z = -\delta_{ns}$  yields the eigenvalues by means of a cubic equation, namely

$$E_{ns}^3 - \frac{\lambda^2 \delta_{ns}^3}{2} (1 + \gamma E_{ns})^2 = 0. \tag{35}$$

This equation has a single positive root, the two others being complex conjugated and thus have to be rejected.

It is interesting to note that the asymptotic limit of  $\delta_{ns}$  as  $n$  get large is given by

$$\delta_{ns} \approx - \left( \frac{3\pi}{2} n \right)^{2/3}, \quad n \geq 10. \tag{36}$$

By inserting this value in equation (35), we readily see that as  $n \rightarrow \infty$  we obtain the limit

$$\lim_{n \rightarrow \infty} E_{ns} = \frac{1}{|\gamma|}. \tag{37}$$

### 3.4. Numerical code

The use of a numerical code has been made to get the eigenvalues of two power-law potentials:  $\alpha = 1/2$  and  $\alpha = 1, \ell \neq 0$ . It prompts us to add a remark concerning the way the Schrödinger equation is solved numerically. The code we are using relies on the behavior of  $r_0$ , the first zero of the reduced wavefunction beyond the origin (remember the boundary conditions  $\Phi(0) = \Phi(\infty) = 0$ ). The quantity  $r_0$  must be a monotonically decreasing function of  $E$ . Considering two solutions of equation (16) for  $E + dE$  and  $E$ , algebraic manipulations lead to

$$\frac{dr_0}{dE} = \frac{-1}{\Phi^2(r_0)} \left[ \int_0^{r_0} \Phi_E^2(r) dr - \gamma \int_0^{r_0} V(r) \Phi_E^2(r) dr \right]. \tag{38}$$

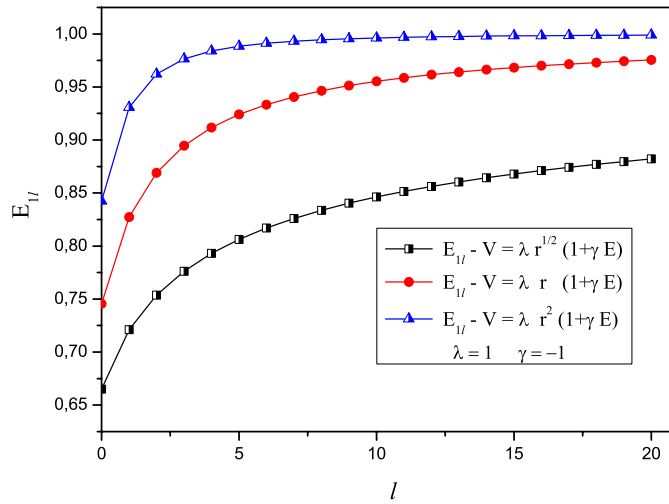
The condition imposed on  $\gamma$  to ensure the density to be positive definite are precisely the ones making this second term the same sign as the first one. In this case, the quantity in the square parenthesis is positive definite, and  $r_0$  is a monotonically decreasing function of  $E$ . Consequently, for power-law potentials, our code can be used by simply replacing  $V(r)$  by  $V(r)(1 + \gamma E)$ . However, for more general potential shapes, one may encounter difficulties with this method.

### 3.5. Saturation of the spectrum

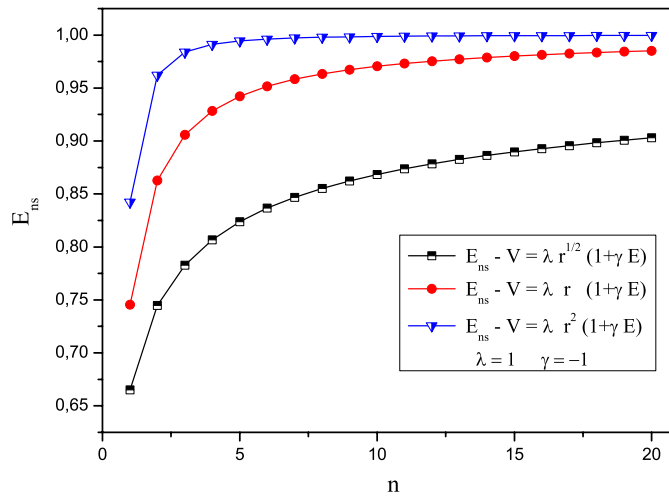
The results obtained for the harmonic oscillator and the linear potential clearly show a saturation effect on the spectrum. The eigenvalues reach an upper bound as the quantum numbers increase. Indeed, such a behavior can be expected for any confining potential dependent on energy. The argument is the following. Consider the potential

$$V(r, E) = \lambda f(r)(1 + \gamma E), \tag{39}$$





**Figure 3.** Behavior of the spectrum of the  $\{1, \ell\}$  states for three different confining shapes of the potential. The upper bound of the spectrum  $\frac{1}{|\gamma|}$  being the same for all three potentials, it shows that the upper limit is reached more rapidly as the power  $\alpha$  of  $r^\alpha$  increases.



**Figure 4.** The same comment as figure 3 for the  $E_{ns}$  spectra.

where  $\lambda$ ,  $f(r)$  and  $E$  are positive definite quantities. Remember as well that for such potentials, the condition of positivity of the density (1) implies  $\gamma \leq 0$ . If an effective coupling constant is defined by

$$\lambda_{\text{eff}} = \lambda(1 + \gamma E_{n\ell}), \tag{40}$$

the largest eigenvalue which can be reached without changing the nature of the confining potential is precisely  $1/|\gamma|$ .

The rapidity of the saturation depends both on  $\gamma$  and on the shape of the potential (here  $\alpha$ ). For the sake of illustration, eigenvalues are displayed as a function of quantum numbers in figures 3 and 4.

In figures 3 and 4, the  $\{1\ell\}$  and the  $\{n0\}$  spectra are displayed for  $\alpha = 0.5, 1.0$  and  $2.0$ , respectively. Here,  $\lambda = 1.0$  and  $\gamma = -1$ . The saturation effect is well underlined: the curves describing the evolution of the eigenvalues with  $\ell$  or  $n$  clearly become flatter as these quantum numbers increase. The way the spectrum reaches its upper limit depends strongly on  $\alpha$ , being the more pronounced as  $\alpha$  is larger.

It is easy to verify that the saturation energy is reached more rapidly as  $|\gamma|$  becomes larger. This can be inferred from the  $1/|\gamma|$  limit. Thus, for large values of  $|\gamma|$ , the whole spectrum is practically degenerated.

#### 4. The equivalent local potential

The equivalent local potentials have been studied in connection with the scattering states. In this context, equivalent local potentials are defined as giving the same asymptotic phase shifts for elastic scattering [18, 19]. To our knowledge, the case for bound states has not been investigated at a formal level. Consequently, this section is devoted to the following question: assuming the spectrum of a non-local potential to be known, is it always possible to find an equivalent local potential producing the same spectrum?

Whereas this is intuitively achievable for a finite set of eigenvalues, no proof exists that it can be extended to the whole spectrum.

The fact that the energy-dependent potentials we have studied reduce to non-local potentials obeying ordinary quantum mechanics rules provides us with a way of tackling this question. Moreover, by considering the Coulomb potential and the harmonic oscillator, we rely on exact (analytical) solutions for an infinite ensemble of states. These starting points are particularly convenient to answer the question of the existence of the local equivalent potential, or at least to show different types of situations. For this purpose, use is made of the method for the inverse problem in the case of discrete states developed in a preceding paper [20]. In particular, conditions for a unique answer have been given in [20, 21].

##### 4.1. The method

Here, the method developed in [20] is briefly recalled. Suppose the eigenvalues to be known, the first step consists in connecting the moments of the ground state density to the excitation energies of the *yrast* levels (the lowest level of each angular momentum). It yields the following recurrent relationships:

$$\langle r^{2\ell} \rangle = \frac{1}{2} \ell(2\ell + 1) \frac{\langle r^{2\ell-2} \rangle}{E_{1\ell} - E_{1s}} f(\ell) \quad (41)$$

The factors  $f(\ell)$  are not known *a priori*. They can be approximated, and then improved by an iterative procedure. For the Coulomb potential and the harmonic oscillator, Bertlmann and Martin have derived an exact expression for  $f(\ell)$  [22]. It will be used here as a first guess. It reads

$$f(\ell) = \left[ 1 - \frac{\ell}{2(\ell + 1)} C(\ell) \right], \quad (42)$$

with

$$C(\ell) = \left[ \frac{E_{(\ell+1)s} + E_{1s} - 2E_{1\ell}}{E_{(\ell+1)s} - E_{1s}} \right]^2. \quad (43)$$

By means of equations (42), (43) and (41) the moments of the ground state density are estimated.

The problem of reconstructing a function from its moments has a long history. In general it has a unique solution if and only if all the moments (integer and non-integer) are known. On the other hand, if only integer moments are fixed, Stieltjes has shown that the solution is by far non-unique [23]. We are precisely facing such a situation, since equations (43) yield only the even moments of the ground state density. However, in the present case, we are looking for densities belonging to the class of square functions  $|\Psi|^2$ , where  $\Psi$  is the solution of the Schrödinger equation for a bound state. In this case, it is sufficient to argue that the density must be a positive definite function decreasing monotonically beyond a given radius. These restrictions ensure the uniqueness of the solution.

Besides the uniqueness, the question remains of how to recover in practice a function from its moments. In the method we have developed, use is made of the formal series expansion of the Fourier transform of the density:

$$F(q) = \frac{1}{2\pi} \int e^{iq\vec{r}} \rho(r) d^3r = \sum_{\ell} (-)^{\ell} \frac{\langle r^{2\ell} \rangle}{(2\ell + 1)!} q^{2\ell}. \quad (44)$$

The expansion is clearly valid only inside the convergence radius. The use of Padé approximants allows us to describe  $F(q)$  beyond the convergence radius. We remind the reader that a Padé approximant is a rational fraction  $P[N, D]$ , where  $N$  and  $D$  are the degree of the numerator and the denominator, respectively. Its coefficients are fitted on the first  $(N + D)$  terms of the series expansion to be extended [24].

Once  $F(q)$  is determined, the ground state density is obtained by inverting the Fourier transform (44). The ground state wavefunction is the square root of the density. The corresponding potential is derived by inverting the Schrödinger equation.

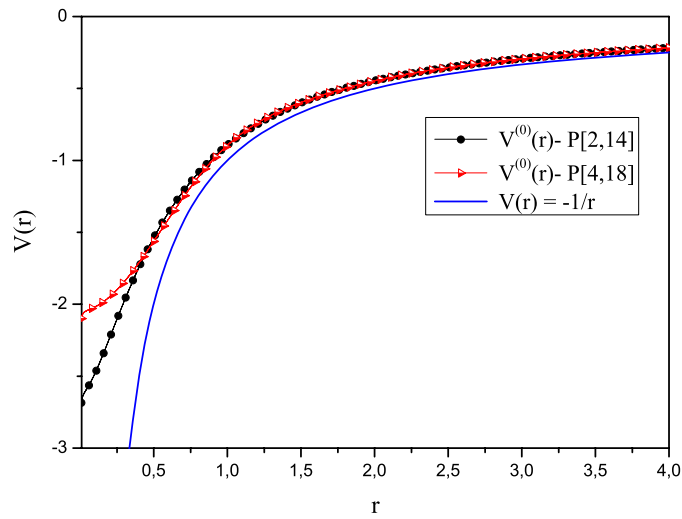
By solving the Schrödinger equation with this potential, the eigenvalues are checked against the original spectrum. This is the essential test. It is also used to calculate new approximated  $f(\ell)$  factors, and to start an iterative procedure. The iterations are stopped once the desired accuracy is reached for the eigenvalues. At a certain step, it may be advantageous to leave the Padé approximants and to work with parametric expressions for the potential.

#### 4.2. The Coulomb potential

The eigenvalues are given by equation (23). They are used to estimate the ground state density moments. The results up to  $\ell = 10$  are displayed in table 1, for both  $f(\ell) = 1$  and  $f(\ell)$  given by equations (42) and (43). Following the procedure stated above, several Padé approximants have been considered. Out of this sample, two approximants,  $P[2,14]$  and  $P[4,18]$ , have been selected as good representatives of what can be achieved in this way. The ground state densities and the corresponding potentials have been derived. The potentials are displayed in figure 5, and compared to the  $-1/r$  potential. Differences appear essentially at small distances.

The validity of the derived potentials is tested by inserting them in the Schrödinger equation and calculating the eigenvalues. At large distances, these potentials have been extrapolated by  $-1/r$ . The two approximants yield equivalent results. The values obtained from  $P[4, 18]$  are listed in table 2, and compared to the exact values. The agreement is satisfactory, the largest deviation being of 4%.

To improve the situation, these first-order potentials can be used to calculate better correction factors  $f(\ell)$ , and start an iterative procedure. On the other hand, improving the results requires also to enlarge the degree  $(N + D)$  of the approximants. However, increasing the degree increases the difficulty of the numerical handling, which becomes rapidly over-complicated. For this reason, at some stage, it is more convenient to play with a parametrized form suggested by the first approximants.



**Figure 5.**  $V(r, E)$ —Coulomb potential: the equivalent potentials  $V^{(0)}(r)$  deduced from the approximants  $P[2, 14]$  and  $P[4, 18]$  are compared to the Coulomb potential.

**Table 1.**  $V(r, E)$ —Coulomb potential: values of the ground state moments  $\langle r^{2\ell} \rangle_{BM}$ ,  $\langle r^{2\ell} \rangle^{(0)}$  and  $\langle r^{2\ell} \rangle_P$  for  $(\lambda = -1, \gamma = 0.5)$  up to  $\ell = 10$ .

$\ell$	$\langle r^{2\ell} \rangle_{BM}$	$\langle r^{2\ell} \rangle^{(0)}$	$\langle r^{2\ell} \rangle_P$
1	$6.4742 \times 10^0$	$4.8556 \times 10^0$	$5.0307 \times 10^0$
2	$1.1144 \times 10^2$	$5.5720 \times 10^1$	$6.3584 \times 10^1$
3	$3.7404 \times 10^3$	$1.1689 \times 10^3$	$1.4780 \times 10^3$
4	$2.0810 \times 10^5$	$3.9018 \times 10^4$	$5.3596 \times 10^4$
5	$1.7371 \times 10^7$	$1.8999 \times 10^6$	$2.7380 \times 10^6$
6	$2.0341 \times 10^9$	$1.2713 \times 10^8$	$1.8376 \times 10^8$
7	$3.1840 \times 10^{11}$	$1.1194 \times 10^{10}$	$1.5393 \times 10^{10}$
8	$6.4246 \times 10^{13}$	$1.2548 \times 10^{12}$	$1.5467 \times 10^{12}$
9	$1.6243 \times 10^{16}$	$1.7449 \times 10^{14}$	$1.8056 \times 10^{14}$
10	$5.0306 \times 10^{18}$	$2.9477 \times 10^{16}$	$2.3833 \times 10^{16}$

After few trials, the following expression has been chosen:

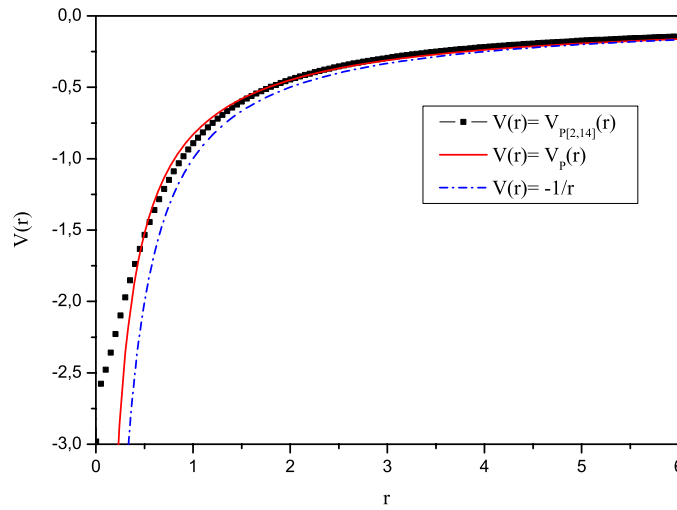
$$V_p(r) = -\frac{V_0(r)}{r^{\alpha(r)}}, \tag{45}$$

with

$$V_0(r) = b + (1 - b) \tanh(kr)^p; \quad \alpha(r) = \alpha_0 + \frac{(1 - \alpha_0)r}{a + r}. \tag{46}$$

The adopted parameter values are  $b = 0.831$ ,  $k = 0.013$ ,  $p = 1.4$ ,  $\alpha_0 = 0.87$  and  $a = 11$ . This form is taken up to  $r = 50$ . Beyond this value, the parametric potential is extrapolated by  $-1/r$ .

The corresponding potential is displayed in figure 6, and is compared with the  $V_{P[2,14]}(r)$  and  $-1/r$  potentials. Near the origin,  $V_p$  behaves like  $-\frac{0.831}{r^{0.875}}$ , which is somewhat less diverging than the Coulomb potential. The comparison with  $V_{P[2,14]}(r)$  underlines one of the difficulties



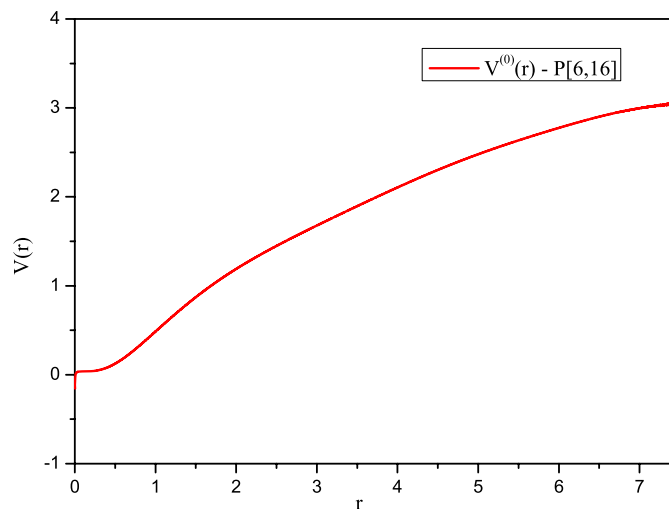
**Figure 6.**  $V(r, E)$ —Coulomb potential: the local equivalent parametric potential is compared to  $V_{P[2,14]}(r)$  and to the Coulomb potential.

**Table 2.**  $V(r, E)$ —Coulomb potential: the first ten eigenvalues  $E_{1\ell}$  of the  $\{1, \ell\}$  states in the case of  $(\lambda = -1, \gamma = 0.5)$ . The exact values are compared to the results obtained with the  $V_{P[2,14]}^{(0)}$  potential, the parametric potential  $V_p(r)$  and the parametric potential extrapolated by  $V(r) = -\frac{1}{r}, r \geq 50 (V_p^{ex}(r))$ . The same is done for the ground state moments  $\langle r^2 \rangle$  and  $\langle r^4 \rangle$ .

$\ell$	$E_{1\ell}$			
	Exact	$V_{P[2,14]}^{(0)}$	$V_p$	$V_p^{ex}$
0	-0.3431	-0.3432	-0.3431	-0.3431
1	-0.1115	-0.1112	-0.1111	-0.1111
2	-0.0527	-0.0549	-0.0530	-0.0530
3	-0.0303	-0.0312	-0.0302	-0.0302
4	-0.0196	-0.0200	-0.0194	-0.0194
5	-0.0137	-0.0139	-0.0136	-0.0136
6	-0.0101	-0.0102	-0.0101	-0.0101
7	-0.0078	-0.0078	-0.0079	-0.0078
8	-0.0061	-0.0062	-0.0064	-0.0062
9	-0.0050	-0.0050	-0.0053	-0.0050
10	-0.0041	-0.0041	-0.0044	-0.0041
$\langle r^2 \rangle$	3.7312	5.0771	5.1757	5.1757
$\langle r^4 \rangle$	38.443	62.351	64.062	64.062

faced with the Padé approximants: the determination of the potential near the origin requires a huge and accurate numerical work. In the present work, it affects essentially the  $\ell = 0$  states, and  $V_p$  constitutes a sufficient approximation for our purpose.

The eigenvalues are listed in table 2. The agreement with the exact values is satisfactory. The slight over-binding found for  $\ell \geq 7$  is due to the fact that  $V_p$  is meeting the  $-\frac{1}{r}$  behavior too slowly. This can be remedied by extrapolating  $V_p(r) = -\frac{1}{r}$  for  $r \geq 50$ . The corresponding eigenvalues are listed in table 2 under  $V_p^{ex}$ .



**Figure 7.**  $V(r, E)$ —harmonic oscillator: the local equivalent potential  $V^{(0)}(r)$  deduced from the approximant  $P[6, 16]$ .

In view of these results, taking into account that at large distances the potential must meet a  $-1/r$  shape, we conclude that a local equivalent potential can be found, which reproduces the whole spectrum. The degree of precision is essentially a question of numerical analysis.

This is not surprising, in a sense, because the non-locality of the original potential affects merely the low lying states. Thus, the problem is not so different from the fit of a spectrum over a finite domain of eigenvalues.

It is interesting to note that, if the spectrum is well reproduced, the ground state wavefunction presents large differences. This is reflected in the values of  $\langle r^2 \rangle$  and  $\langle r^4 \rangle$  quoted in table 2. The extension of the wavefunction of the local equivalent potential is much larger than the one of the original wavefunction.

#### 4.3. The harmonic oscillator case

The situation is radically different in the case of the harmonic oscillator, and probably for all confining potentials.

The eigenvalues are given by the positive roots of equation (29). They are used to obtain the first estimate of  $f(\ell)$  and the ground state density moments. They are displayed up to  $\ell = 10$  in table 3. These moments are considered to build Padé approximants to  $F(q)$ . Among various possibilities, we have retained the  $P[6, 16]$  fraction, which illustrates the situation very well. The corresponding potential is displayed in figure 7. Close to the origin, the shape reminds us of the harmonic oscillator but as  $r$  increases, the slope bends and the shape looks logarithmic. Such a behavior is actually expected, since the saturation of the spectrum implies the potential to tend to a constant.

The spectrum has been calculated by extrapolating this potential beyond  $r = 7$  by two expressions:

$$V_1(r) = 1.3916 \log(0.1 + r); \quad V_2(r) = r^{\alpha(r)} \quad \text{with} \quad \alpha(r) = 0.223 - 0.15e^{-0.3r}. \quad (47)$$

The results are displayed in table 4, and compared to the exact values. The agreement is no better than a few percent but it is sufficient to underline the main problem. The local

**Table 3.**  $V(r, E)$ —Harmonic oscillator: values of the ground state moments  $\langle r^{2\ell} \rangle_{BM}$ ,  $\langle r^{2\ell} \rangle^{(0)}$  and  $\langle r^{2\ell} \rangle_P$  for  $(\lambda = 0.5, \gamma = -0.25)$  up to  $\ell = 10$ .

$\ell$	$\langle r^{2\ell} \rangle_{BM}$	$\langle r^{2\ell} \rangle^{(0)}$	$\langle r^{2\ell} \rangle_P$
1	$2.5291 \times 10^0$	$2.5174 \times 10^0$	$2.4388 \times 10^0$
2	$1.2111 \times 10^1$	$1.1768 \times 10^1$	$1.1385 \times 10^1$
3	$9.1687 \times 10^1$	$8.4171 \times 10^1$	$8.2837 \times 10^1$
4	$1.0013 \times 10^3$	$8.3327 \times 10^2$	$8.4974 \times 10^2$
5	$1.4892 \times 10^4$	$1.0741 \times 10^4$	$1.2059 \times 10^4$
6	$2.8977 \times 10^5$	$1.7309 \times 10^5$	$3.3170 \times 10^5$
7	$7.1557 \times 10^6$	$3.3896 \times 10^6$	$3.3893 \times 10^7$
8	$2.1896 \times 10^8$	$7.8987 \times 10^7$	$6.6277 \times 10^9$
9	$8.1417 \times 10^9$	$2.1555 \times 10^9$	$1.4333 \times 10^{12}$
10	$3.6198 \times 10^{11}$	$6.8021 \times 10^{10}$	$3.1388 \times 10^{14}$

**Table 4.**  $V(r, E)$ —harmonic oscillator: the first ten eigenvalues  $E_{1\ell}$  of the  $\{1, \ell\}$  states in the case of  $(\lambda = 0.5, \gamma = -0.25)$ . The exact values are compared to the results obtained with  $V_1^{(0)}(r)$  and  $V_2^{(0)}(r)$  as well as with  $V^{(1)}(r)$ . The same is done for the ground state moments  $\langle r^2 \rangle$  and  $\langle r^4 \rangle$ .

$\ell$	$E_{1\ell}$	$E_{1\ell}^{(0)}$		$E_{1\ell}^{(1)}$
	Exact	$V_1^{(0)}$	$V_2^{(0)}$	$V^{(1)}$
0	1.2449	1.2469	1.2469	1.2467
1	1.8380	1.8316	1.8319	1.8359
2	2.2891	2.2807	2.2840	2.2981
3	2.6318	2.6368	2.6535	2.6532
4	2.8932	2.8963	2.9291	2.9155
5	3.0938	3.0922	3.0998	3.0931
6	3.2492	3.2645	3.2207	3.2190
7	3.3709	3.4256	3.3228	3.3225
8	3.4672	3.5763	3.4136	3.4135
9	3.5442	3.7158	3.4957	3.4956
10	3.6066	3.8438	3.5703	3.5703
$\langle r^2 \rangle$	2.0294	2.5222	2.5214	2.5064
$\langle r^4 \rangle$	6.7820	11.825	11.809	11.442

equivalent potential behaves at large distances as a confining potential. Thus, its eigenvalues are constantly increasing. The saturation of the spectrum cannot be reached in this way.

The procedure can be iterated by calculating improved  $f(\ell)$  from these first two potentials. However, the improvement of the fit is not so spectacular. Thus, it will not be discussed further.

There is, however, one way to reproduce the energy differences of the discrete spectrum. This can be achieved by shifting the whole spectrum by  $-\frac{1}{|\gamma|}$ . The problem thus resembles the Coulomb potential case, with the saturation energy shifted to zero.

Based on the experienced gained with the Coulomb potential, we have adopted the following parametrized expression:

$$V_p(r) = -\frac{V_0(r)}{r^{\alpha(r)}}, \tag{48}$$

**Table 5.**  $V(r, E)$ —harmonic oscillator: the first ten eigenvalues  $E_{1\ell}$  of the  $\{1, \ell\}$  states in the case of  $(\lambda = 0.5, \gamma = -0.25)$ . Exact values are compared to the results obtained with the parametric potential  $V_P(r)$  and the parametric potential extrapolated by  $V(r) = -\frac{1}{r}, r \geq 10: (V_P^{ex}(r))$ . The same is done for the ground state moments  $\langle r^2 \rangle$  and  $\langle r^4 \rangle$ .

$\ell$	$E'_{1\ell}$		
	$V_{\text{exact}}$	$V_P$	$V_P^{ex}$
0	-2.7551	-2.7577	-2.7577
1	-2.1620	-2.1596	-2.1596
2	-1.7109	-1.7360	-1.7360
3	-1.3682	-1.4045	-1.4045
4	-1.1068	-1.1358	-1.1359
5	-0.9062	-0.9153	-0.9161
6	-0.7508	-0.7333	-0.7403
7	-0.6291	-0.5832	-0.6170
8	-0.5328	-0.4594	-0.5340
9	-0.4558	-0.3577	-0.4645
10	-0.3934	-0.2746	-0.4012
$\langle r^2 \rangle$	2.0294	2.4388	2.4388
$\langle r^4 \rangle$	6.7820	11.387	11.386

with

$$V_0(r) = 3.37 + \frac{0.4}{(1+r^2)^2}; \quad \alpha(r) = 0.3 + 0.12 \log(1 + 0.25r^2). \quad (49)$$

The corresponding eigenvalues are displayed in table 5, and compared to the exact values.

The agreement is quite satisfactory. It means that if the energy differences between levels are the quantities to be reproduced, then this task is achievable for the whole spectrum as for the Coulomb potential.

However, it is clear that the potential (48) tends to zero as  $r \rightarrow \infty$ , and thus it admits states in the continuum, which are absent in the original potential. Moreover, the ground state wavefunction is now characteristic of the Coulomb case, namely it has an exponential decay. This contrasts with wavefunctions of confining potentials. This is reflected in the ground state moments. As shown in table 3, the values of  $\langle r^{2\ell} \rangle_P$  are sensibly larger than  $\langle r^{2\ell} \rangle_{BM}$  beyond  $\ell = 6$ .

In conclusion, energy-dependent confining potentials have spectra which cannot be reproduced by a local equivalent potential over the entire energy domain. This example puts limits on the possibility of finding local equivalent potential.

Note that the calculated values of  $\langle r^2 \rangle$  and  $\langle r^4 \rangle$  in the ground state show the extension of the ground state wavefunction of the local equivalent potential to be larger than that of the original potential. In this respect, the situation is similar to the one found with the Coulomb potential. In fact, it should be the same for any non-local potential, as shown by the following arguments.

The recurrence relationships (41) are actually derived from some rules (see [25]). Non-local potentials bring corrections to the sum rules, with respect to the local potential, which diminish the sum rule values. Consequently, the ground state moments of a non-local potential are expected to be smaller than those of the local equivalent potential.



## 5. Conclusions

The present work is devoted to the study of energy-dependent potentials. As stated in the introduction, they constitute a way to include nonlinear effects in the Schrödinger equation. A linear energy dependence has been chosen, since it leads to a coherent theory.

To become acquainted with the handling of nonlinear effects, the solutions of the Schrödinger equation have been given for power-law potentials with  $\alpha = -1, 1/2, 1$  and  $2$ . The radial shape is simply multiplied by  $(1 + \gamma E_{nl})$ . The coherence of the theory requires  $\gamma$  to be positive for attractive potentials and negative for confining potentials, respectively. Formally, the solutions resemble that of the ordinary cases ( $\gamma = 0$ ) except that the equations determining the eigenvalues are not linear. In such a case, it is important to verify that only a single root has to be retained.

In the case of numerical solutions of the Schrödinger equation, the very same conditions ensuring the positivity of the density allows the use of the codes used in the case of local potentials. It amounts to replace  $V(r)$  by  $V(r)(1 + \gamma E)$  in the codes. At the same time, it proves that the calculated wavefunction corresponds to a unique eigenvalue.

In general, the energy dependence results in the compression of the spectrum. For the Coulomb potential ( $\alpha = -1$ ), the ground state is less bound as  $\gamma$  increases. Confining potentials are subject to a saturation effect: as the quantum numbers increase, the eigenvalues reach an upper bound.

Finally, since the wave equation with a linear energy dependence in the potential can be reduced to an ordinary Schrödinger equation with a non-local potential, it gives an opportunity to discuss the question of the local equivalent potential. Moreover, the fact that complete analytical solutions exist for the Coulomb potential and the harmonic oscillator provides us with the necessary ingredients to solve the so-called inverse problem from the discrete spectrum. Here, we apply a method developed in a previous work [20].

A local equivalent potential can be found, which reproduces the whole spectrum in the case of the Coulomb potential. The situation is different for the harmonic oscillator. Confining potentials undergo a saturation effect, which can be reproduced only by a shift of the saturation energy to zero. But at the same time, it introduces continuum states, not present in the original potential. Thus, strictly speaking, it is not possible in this case to find a local equivalent potential reproducing the whole spectrum.

Finally, we note that the moments of the ground state density are larger for the local equivalent potential than for the original non-local potential. We conjecture this to be a general consequence of the non-locality of the potential. Our argument is based on the fact that the connections between the ground state moments and the spectrum are derived from sum rules, and that the sum rule values are smaller for non-local potentials.

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