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Renormalization-group solutions for Yukawa potential

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Abstract. The self-similar renormalization group is used to obtain expressions for the spectrum of the Hamiltonian with the Yukawa potential. The critical screening parameter above which there are no bound states is also obtained by this method. The approach presented illustrates that one can achieve good accuracy without involving extensive numerical calculations, but invoking instead the renormalization-group techniques.

1. Introduction

Renormalization-group techniques are widely used in quantum field theory, statistical mechanics, and solid-state physics. Their usage in atomic physics is less customary. The aim of the present paper is to show how renormalization-group ideas can be applied for calculating the spectra of quantum-mechanical Hamiltonians with realistic potentials.

As a model for illustration we opt for a Hamiltonian with the Yukawa potential. This choice is based on the special role of this potential in different branches of physics. In plasma physics it is known as the Debye–Hückel potential, in solid-state physics and atomic physics it is called the Thomas–Fermi or screened Coulomb potential, and in nuclear physics one terms it the Yukawa potential. Among recent important applications of this potential we may mention its use in the models describing the metal–insulator transition [1].

The problem of finding the energy levels for the Yukawa potential has received a lot of attention in the literature. Several approaches have been used for solving this problem: the simple variational procedure [2], use of atomic orbitals with a set of fitting parameters [3], Rayleigh–Schrödinger perturbation theory [4, 5], the method of potential envelopes [6–9], an iterative procedure [10], and different numerical calculations [11–14].

In this paper we demonstrate how the problem can be treated by employing the self-similar approximation theory [15–19] based on the ideas of the renormalization-group and dynamical theory. The outline of the paper is as follows. In section 2 we sketch the main steps of the procedure using the self-similar renormalization group. We present only those formulae that are necessary for understanding the following calculations; all details and the mathematical foundations can be found in [15–19]. In section 3 we apply the approach to the Schrödinger equation with the Yukawa potential. In section 4 we obtain the sequence of renormalized energies. The convergence of this sequence is governed by control functions defined from the minimum of the multiplier. In section 5 the procedure is applied to calculating the renormalized critical screening parameter. We emphasize that we are presenting here an analytical method, not relying on heavy numerical calculations. Despite its analytical nature, the method gives quite good accuracy for the critical screening parameter obtained.

2. Self-similar renormalization

We give here the general sketch of the procedure [15–19], without specifying the nature of the functions involved. Suppose a function $f(x)$ is defined by a complicated equation that is being solved approximately. Employing a perturbative algorithm, we obtain a sequence of approximations, $\{F_k\}_{k=0}^{\infty}$, for the sought function $f(x)$. To make the sequence convergent, we incorporate into the approximations $F_k = F_k(x, u_k)$, with $k = 0, 1, 2, \dots$, a set of control functions $u_k = u_k(x)$, so that the sequence $\{f_k(x)\}_{k=0}^{\infty}$ of the approximations

$$f_k(x) \equiv F_k(x, u_k(x)) \quad (1)$$

is convergent.

We make the change of variables by defining a function $x_k(f)$ through the equation

$$F_0(x, u_k(x)) = f \quad x = x_k(f) \quad (2)$$

in which f is the new variable. With this change of variables, equation (1) yields

$$y_k(f) \equiv f_k(x_k(f)). \quad (3)$$

The transformation inverse to equation (3) is

$$f_k(x) = y_k(F_0(x, u_k(x))). \quad (4)$$

We now construct an approximation cascade $\{y_k\}$ by requiring the self-similarity relation

$$y_{k+p}(f) = y_k(y_p(f)). \quad (5)$$

The trajectory $\{y_k(f)\}_{k=0}^{\infty}$ of this approximation cascade is, according to equations (3) and (4), bijective to the sequence $\{f_k(x)\}_{k=0}^{\infty}$ of approximations in equation (1). Embedding the approximation cascade into an approximation flow and integrating the evolution equation for the latter, we obtain the evolution integral

$$\int_{f_k}^{f_{k+1}^*} \frac{df}{v_k(f)} = t_k^* \quad (6)$$

in which $f_k = f_k(x)$ is a given approximation, $f_k^* = f_k^*(x)$ is a renormalized self-similar approximation, and

$$v_k(f) = F_{k+1}(x_k, u_k) - F_k(x_k, u_k) + (u_{k+1} - u_k) \frac{\partial}{\partial u_k} F_k(x_k, u_k) \quad (7)$$

is the cascade velocity, where $x_k = x_k(f)$ and $u_k = u_k(x_k(f))$. The right-hand side of equation (6), that is t_k^* , is the minimal time necessary for reaching the renormalized approximation $f_{k+1}^*(x)$.

A fixed point $y_k^*(f)$ of the approximation cascade represents, by construction, the sought function $f(x)$ which can be obtained from transformation (4). At the fixed point the cascade velocity $v_k(f) \rightarrow 0$ as $k \rightarrow \infty$. If the cascade velocity is not zero exactly, but only approximately, then we do not have an actual fixed point, but a quasi-fixed point. For instance, assuming that $v_k(f) \approx 0$ and $F_{k+1} \approx F_k$, from equation (7) we have

$$(u_{k+1} - u_k) \frac{\partial}{\partial u_k} F_k(x, u_k) = 0 \quad (8)$$

which is a quasi-fixed-point condition.

The convergence of the approximation sequence $\{f_k(x)\}_{k=0}^{\infty}$ is equivalent to the stability of the cascade trajectory $\{y_k(f)\}_{k=0}^{\infty}$. The stability of the latter can be analysed by defining the multipliers

$$\mu_k(f) \equiv \frac{\partial}{\partial f} y_k(f) \quad (9)$$

and

$$m_k(x) \equiv \frac{\delta F_k(x, u_k(x))}{\delta F_0(x, u_k(x))}. \tag{10}$$

These multipliers are images of each other, being related by the transformations

$$\mu_k(f) = m_k(x_k(f)) \quad m_k(x) = \mu_k(F_0(x, u_k(x))). \tag{11}$$

The trajectory is locally stable when

$$|m_k(x)| \leq 1 \quad |\mu_k(f)| \leq 1. \tag{12}$$

The multipliers (9) and (10) describe the local stability, at the step k , of the cascade trajectory with respect to the variation of initial conditions. This type of local multiplier can be called a quasi-local multiplier [19]. Another type of local multiplier defined as

$$m_k^*(x) \equiv \frac{m_k(x)}{m_{k-1}(x)}$$

characterizes the local stability, at the step k , with respect to the variation of the point $k - 1$. The latter multiplier can be termed ultra-local.

Recall that control functions are introduced so as to provide the convergence of the approximation sequence $\{f_k(x)\}_{k=0}^\infty$, that is, the stability of the cascade trajectory $\{y_k(f)\}_{k=0}^\infty$. This suggests a way for the practical definition of control functions. The local multiplier (10) may be written as

$$m_k(x) = M_k(x, u_k(x)) \tag{13}$$

with

$$M_k(x, u) = \frac{\partial F_k(x, u)}{\partial u} \bigg/ \frac{\partial F_0(x, u)}{\partial u}. \tag{14}$$

To produce the maximal stability of the cascade trajectory, i.e. the fastest convergence of the approximation sequence, for each fixed value of x , we have to require the minimum of the absolute value for the multiplier (13) with respect to the control function $u_k(x)$. In other words, the principal of maximal stability is the condition for the minimum of the multiplier modulus,

$$\min_u |M_k(x, u)| = |M_k(x, u_k(x))|. \tag{15}$$

This condition gives us a constructive definition of control functions.

3. Yukawa potential

Now we illustrate how the scheme of section 2 applies in the calculation of the eigenvalues of the radial Hamiltonian

$$H = -\frac{1}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} - \frac{A}{r} e^{-\alpha r}$$

with the Yukawa potential.

It is convenient to pass to dimensionless quantities by scaling the above Hamiltonian and reducing it to the form

$$H = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{e^{-\alpha r}}{r}. \tag{16}$$

Here $r \in [0, \infty)$; $l = 0, 1, 2, \dots$; and α is a positive constant called the screening parameter. To return back to dimensional quantities one has to make the following substitutions:

$$r \rightarrow mA r \quad \alpha \rightarrow \frac{\alpha}{mA} \quad H \rightarrow \frac{H}{mA^2}.$$

Write Hamiltonian (16) as the sum $H \equiv H_0 + \Delta H$, with the first term being the Hamiltonian

$$H_0 = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{u}{r} \quad (17)$$

with a Coulomb-type potential, where u is a yet unknown quantity which will later generate control functions.

Employing some variant of perturbation theory in powers of the perturbation

$$\Delta H \equiv H - H_0 = \frac{u - e^{-\alpha r}}{r} \quad (18)$$

we may construct a sequence of approximate eigenvalues, E_k , and eigenfunctions, ψ_k , respectively,

$$E_k \equiv E_{nl}^{(k)}(\alpha, u) \quad \psi_k \equiv \psi_{nl}^{(k)}(r, u) \quad (19)$$

where $k = 0, 1, 2, \dots$ enumerates approximations, while $n = 0, 1, 2, \dots$ and $l = 0, 1, 2, \dots$ are the quantum numbers labelling the energy levels. For the initial approximation one has the spectrum

$$E_0 = -\frac{u^2}{2(n+l+1)^2} \quad (20)$$

and the wavefunction

$$\begin{aligned} \psi_0 = & \left[\frac{n!u}{(n+2l+1)!} \right]^{1/2} \frac{1}{n+l+1} \left(\frac{2ur}{n+l+1} \right)^{l+1} \exp\left(-\frac{ur}{n+l+1}\right) \\ & \times L_n^{2l+1}\left(\frac{2ur}{n+l+1}\right) \end{aligned} \quad (21)$$

in which

$$L_n^l(r) = \sum_{m=0}^n \frac{\Gamma(n+l+1)(-r)^m}{\Gamma(m+l+1)(n-m)!m!}$$

is an associate Laguerre polynomial.

To find the subsequent approximations, we could use the Rayleigh–Schrödinger perturbation theory. However, this would involve the following complication. The whole spectrum of the Hamiltonian (16) contains, in addition to discrete levels, the continuous part. Therefore, we would have to deal with, besides the summation over discrete levels, the integration over continuous ones.

To avoid this complication, when we are interested only in discrete levels, we may employ the Dalgarno–Lewis perturbation theory [20]. Then, for the k -approximation one writes

$$\begin{aligned} E_k &= E_0 + \sum_{p=1}^k \Delta E_p \\ \psi_k &= \psi_0 + \sum_{p=1}^k \Delta \psi_p. \end{aligned} \quad (22)$$

The first correction for the eigenvalues is

$$\Delta E_1 = (\psi_0, \Delta H \psi_0) \quad (23)$$

and the first correction to the eigenfunction is a solution to the equation

$$(H_0 - E_0)\Delta\psi_1 = (\Delta E_1 - \Delta H)\psi_0. \quad (24)$$

Solving the Dalgarno equation (24), one may calculate the second correction to the eigenvalues,

$$\Delta E_2 = (\Delta\psi_1, \Delta H \psi_0) \quad (25)$$

and so on.

The Dalgarno equation (24) is a non-homogeneous equation whose solution can be written as the sum of the general solution to the corresponding homogeneous equation plus a particular solution to the non-homogeneous equation. The solution to the homogeneous equation is, as is evident, proportional to ψ_0 . So we may set

$$\Delta\psi_1 = C\psi_0 + \varphi \quad (26)$$

with the proportionality constant C defined by the normalization condition $(\psi_k, \psi_k) = 1$, and the function φ being a particular solution to the non-homogeneous equation

$$(H_0 - E_0)\varphi = (\Delta E_1 - \Delta H)\psi_0. \quad (27)$$

From the normalization condition $(\psi_1, \psi_1) = 1$, for the function $\psi_1 = \psi_0 + \Delta\psi_1$, omitting the second-order term, one has

$$(\psi_0, \Delta\psi_1) = 0. \quad (28)$$

With equation (26), this gives

$$C = -(\psi_0, \varphi). \quad (29)$$

Following the scheme described, with the notation

$$\beta \equiv \frac{\alpha}{2u}(n+l+1) \quad (30)$$

we obtain the first correction for the eigenvalues of bound states,

$$\Delta E_1 = \frac{u^2 I_0 - u I_\beta}{(n+l+1)^2} \quad (31)$$

where the integral

$$I_\beta \equiv \frac{n!}{(n+2l+1)!} \int_0^\infty r^{2l+1} e^{-(1+\beta)r} [L_n^{2l+1}(r)]^2 dr$$

can be expressed as

$$I_\beta = \frac{(\beta-1)^n}{(\beta+1)^{n+2l+2}} \mathcal{P}_n^{2l,0} \left(\frac{\beta^2+1}{\beta^2-1} \right)$$

through the Jacobi polynomials

$$\begin{aligned} \mathcal{P}_n^{k,p}(x) &= \frac{(-1)^n}{2^n n!} (1-x)^{-k} (1+x)^{-p} \frac{d^n}{dx^n} [(1-x)^{n+k} (1+x)^{n+p}] \\ &= \frac{1}{2^n} \sum_{m=0}^n C_{n+k}^m C_{n+p}^{n-m} (x-1)^{n-m} (x+1)^m \end{aligned}$$

having the properties

$$\mathcal{P}_n^{k,p}(1) = C_{n+k}^n \quad \mathcal{P}_n^{k,p}(-1) = (-1)^n C_{n+p}^n \quad C_n^m \equiv \frac{n!}{(n-m)!m!}.$$

Another integral in equation (31) is

$$I_0 \equiv \lim_{\beta \rightarrow 0} I_\beta = 1.$$

In this way, the first approximation $E_1 = E_0 + \Delta E_1$ becomes

$$E_1 = \frac{u^2 - 2uI_\beta}{2(n+l+1)^2} \tag{32}$$

where

$$I_\beta = \frac{1}{(1+\beta)^{2n+2l+2}} \sum_{m=0}^n C_{n+2l+1}^m C_n^{n-m} \beta^{2m}.$$

For the ground-state level, when $n = l = 0$ and $\beta = \alpha/2u$, equation (32) reduces to

$$E_1 = -u^2 \left(\frac{1}{2} - \sigma \right) \tag{33}$$

where the notation

$$\sigma \equiv 1 - \frac{4u}{(2u + \alpha)^2} \tag{34}$$

is introduced.

The ground state plays a special role defining, when it becomes zero, the critical screening parameter α_c , above which there are no bound states. Therefore, in what follows we consider the ground state.

Equation (27), with

$$E_0 = -\frac{u^2}{2} \quad \psi_0 = 2u^{3/2}r e^{-ur} \tag{35}$$

can be written as

$$\left(-\frac{1}{2} \frac{d^2}{dr^2} - \frac{u}{r} + \frac{u^2}{2} \right) \varphi = \left(\sigma u^2 - \frac{u}{r} + \frac{e^{-\alpha r}}{r} \right) \psi_0. \tag{36}$$

The solution to equation (36) must be a bounded function, $|\varphi(r)| < \infty$, for all $r \in [0, \infty]$.

Let us present φ as the product

$$\varphi(r) = \psi_0(r)g(ur)$$

in which the second factor satisfies the equation

$$\frac{d}{dr}g(r) = \rho(r)\frac{e^{2r}}{r^2}$$

where $\rho(r)$ is to be defined from equation (36), which yields

$$\frac{d\rho}{dr} = (1 - \sigma r)2r e^{-2r} - \frac{2r}{u} \exp\left(-\frac{2u + \alpha}{u}r\right).$$

The latter equation gives

$$\rho(r) = \left[\sigma r^2 + (\sigma - 1) \left(r + \frac{1}{2} \right) \right] e^{-2r} + \frac{1 - \sigma}{2} \left(1 + \frac{2u + \alpha}{u}r \right) \exp\left(-\frac{2u + \alpha}{u}r\right) + C_1$$

with an integration constant C_1 . The equation for $g(r)$ results in

$$g(ur) = \sigma ur + (1 - \sigma) \left[\frac{1 - e^{-\alpha r}}{2ur} - \ln(ur) + \text{Ei}(-\alpha r) \right] + C_1 \left[2 \text{Ei}(2ur) - \frac{e^{2ur}}{ur} \right] + C_2$$

where C_2 is an integration constant and

$$\text{Ei}(ar) = \int_{-\infty}^r \frac{e^{ax}}{x} dx$$

is the exponential-integral function.

The boundness of φ requires that $C_1 = 0$. The additive term containing a function proportional to ψ_0 should be omitted in φ , since such a term has already been included in equation (26). The latter means that we have to put $C_2 = 0$. As a result we obtain

$$\varphi(r) = \sqrt{u} e^{-ur} \{ 2\sigma(ur)^2 + (1 - \sigma)[1 - e^{-\alpha r} - 2ur \ln(ur) + 2ur \text{Ei}(-\alpha r)] \}. \tag{37}$$

For the normalization constant in equation (29) we find

$$C = -\frac{3}{2}\sigma + (1 - \sigma) \left(\frac{\alpha}{2u + \alpha} - \ln \frac{2\alpha}{2u + \alpha} - \gamma_E \right) \tag{38}$$

with the Euler constant $\gamma_E = 0.577\,215$.

After finding function (26), we can calculate the second correction (25), which yields

$$\Delta E_2 = u^2 J_1 - u J_2 \tag{39}$$

where

$$J_1 = \lim_{v \rightarrow 0} J_2(v) \quad J_2 = J_2(\beta)$$

with $\beta = \alpha/2u$, and

$$J_2(v) = 2 \int_0^\infty \left\{ 2Cr + 2\sigma r^2 + (1 - \sigma) \left[1 - e^{-\alpha r/u} - 2r \ln r + 2r \text{Ei}\left(-\frac{\alpha r}{u}\right) \right] \right\} e^{-2(1+v)r} dr.$$

Thus, for the second approximation for the energy we obtain

$$E_2 = E_1 + u^2 J_1 - u J_2 \tag{40}$$

where

$$J_1 = -\frac{\sigma}{2} + \frac{1 - \sigma}{1 + \beta} \beta$$

$$J_2 = -u(1 - \sigma) \frac{\sigma(1 + 3\beta)}{2(1 + \beta)} + u(1 - \sigma)^2 \left[\frac{(1 + 3\beta + \beta^2)\beta}{(1 + \beta)(1 + 2\beta)} + \ln \frac{(1 + \beta)^2}{1 + 2\beta} \right].$$

4. Renormalized energy

From the results of the previous section we derive the following sequence of approximations for the energy:

$$E_0 = -\frac{u^2}{2}$$

$$E_1 = E_0 + u^2 - \frac{4u^3}{(2u + \alpha)^2}$$

$$E_2 = E_1 - \frac{u^2}{2} + \frac{2u^3}{(2u + \alpha)^2} + \frac{4u^3\alpha}{(2u + \alpha)^3} + \frac{2u^3(2u^2 + 5u\alpha - 2\alpha + 3\alpha^2)}{(u + \alpha)(2u + \alpha)^3} - \frac{8u^4(2u^2 + 5u\alpha + 4\alpha^2)}{(u + \alpha)(2u + \alpha)^5} - \frac{16u^4}{(2u + \alpha)^4} \ln \frac{(2u + \alpha)^2}{4u(u + \alpha)}. \tag{41}$$

For the multiplier defined in equation (14) we have

$$M_k(\alpha, u) = \frac{\partial E_k(\alpha, u)}{\partial u} \bigg/ \frac{\partial E_0(\alpha, u)}{\partial u}. \quad (42)$$

Substituting here the derivatives

$$\begin{aligned} \frac{\partial E_0}{\partial u} &= -u \\ \frac{\partial E_1}{\partial u} &= u - \frac{12u^2}{(2u + \alpha)^2} + \frac{16u^3}{(2u + \alpha)^3} \end{aligned}$$

following from the sequence (41), we find

$$M_1(\alpha, u) = -\frac{8u^3 - 4(2 - 3\alpha)u^2 - 6\alpha(2 - \alpha)u + \alpha^3}{(2u + \alpha)^3}. \quad (43)$$

The control function $u(\alpha) = u_1(\alpha)$ is to be defined from the principle of maximal stability (15). To this end, we first try the equation

$$M_1(\alpha, u) = 0 \quad (44)$$

which gives

$$8u^3 - 4(2 - 3\alpha)u^2 - 6\alpha(2 - \alpha)u + \alpha^3 = 0. \quad (45)$$

This cubic equation has three roots of which we have to select a real one satisfying the asymptotic condition

$$\lim_{\alpha \rightarrow 0} u(\alpha) = 1.$$

The latter implies that if the screening parameter tends to zero, so that the Yukawa potential transforms into the Coulomb one, then one must return to the exact solution known for the Coulomb potential. Really, under $\alpha \rightarrow 0$ and $u \rightarrow 1$, from the sequence in equation (41) it follows that $E_k \rightarrow -\frac{1}{2}$ for all k . Equation (45), with this asymptotic condition, yields the control function

$$u(\alpha) = \frac{1}{3} - \frac{\alpha}{2} + \frac{2}{3} \sqrt{1 + \frac{3}{2}\alpha} \cos \frac{\varphi}{3} \quad (46)$$

in which

$$\varphi = \begin{cases} \varphi^* & \varphi^* \geq 0, 0 \leq \alpha \leq (3 + \sqrt{57})/18 \\ \pi - \varphi^* & \varphi^* \leq 0, (3 + \sqrt{57})/18 \leq \alpha \leq \alpha_0 \end{cases}$$

where

$$\varphi^* = \arctan \frac{3\alpha\sqrt{3(3 + 20\alpha - 27\alpha^2)}}{4 + 9\alpha - 27\alpha^2}$$

and the upper value of the screening parameter, below which equation (45) possesses a solution, is

$$\alpha_0 \equiv \frac{10 + 7\sqrt{7}}{27} = 1.056306. \quad (47)$$

Thus, solution (46) exists only in the interval $0 \leq \alpha \leq \alpha_0$. For $\alpha > \alpha_0$, equation (45) has no real solutions satisfying the derived asymptotic condition.

For $\alpha > \alpha_0$ we need to find a minimum of the multiplier (43), which is not necessarily zero. This can be done by solving the equation

$$\frac{\partial}{\partial u} M_1(\alpha, u) = 0 \quad (48)$$

which results in the control function

$$u(\alpha) = \left(\frac{\sqrt{7}}{2} - 1 \right) \alpha = 0.322\,876\alpha. \quad (49)$$

One may note that when equation (44) has a solution, then the procedure is similar to renormalizing perturbative terms by means of a variational optimization [21–26]. However, as is shown above, this equation does not always possess physically reasonable solutions, while the principle of maximal stability (15) always provides us with a solution defining a control function. Therefore, this principle is more general than the simple variational procedure.

Substituting the found control function into the approximations in the sequence (41), we get the renormalized expressions

$$e_k(\alpha) \equiv E_k(\alpha, u_k(\alpha)). \quad (50)$$

For example, when $\alpha \leq \alpha_0$, we have

$$e_1(\alpha) = -\frac{u^2(2u - \alpha)}{2(2u + 3\alpha)} \quad (51)$$

$$e_2(\alpha) = -\frac{u^2}{2} \left[\frac{8u^4 + 16u^3\alpha - 2u^2\alpha^2 - 10u\alpha^3 + \alpha^4}{2u(u + \alpha)(2u + 3\alpha)^2} + 2 \left(\frac{2u + \alpha}{2u + 3\alpha} \right)^2 \ln \frac{(2u + \alpha)^2}{4u(u + \alpha)} \right]. \quad (52)$$

Respectively, for $\alpha > \alpha_0$, we have to substitute the control function (49) into equation (41).

The self-similar approximation for the energy is to be defined from the evolution integral (6). When no additional constraints are imposed, the minimal number of steps for reaching a quasi-fixed point is, clearly, one, $t_k^* = 1$. In the interval $0 \leq \alpha \leq \alpha_0$, the cascade velocity, given by equation (7), is

$$v_1(f) = e_2(\alpha(f)) - e_1(\alpha(f)) \quad (53)$$

where the function $\alpha(f)$, according to equation (2), is defined by the equation

$$E_0(\alpha, u(\alpha)) = -\frac{1}{2}u^2(\alpha) = f \quad (54)$$

resulting in $\alpha = \alpha(f)$. For the evolution integral (6), we have

$$\int_{e_1}^{e_2^*} \frac{df}{v_1(f)} = 1 \quad (55)$$

where $e_1 = e_1(\alpha)$ and $e_2^* = e_2^*(\alpha)$.

We have calculated the values of the renormalized energies $e_1(\alpha)$, $e_2(\alpha)$ and $e_2^*(\alpha)$ as functions of the screening parameter α . To characterize the accuracy of these approximations, it is convenient to introduce the maximal percentage errors

$$\varepsilon_k \equiv \max_{\alpha} \left[\frac{e_k(\alpha) - e(\alpha)}{|e(\alpha)|} \right] \times 100\%$$

where $e(\alpha)$ is an exact value of the energy. Notice that this definition of the maximal error has sense only when $e(\alpha)$ is not close to zero. In our case this definition works for $0 \leq \alpha \leq \alpha_0$. For $\alpha > \alpha_0$, when $e(\alpha) \rightarrow 0$, it is possible to redefine the maximal error by shifting the definition of the energy by a constant [27].

The maximal percentage error, defined as is explained above, is 2% for $e_1(\alpha)$ and for $e_2(\alpha)$ and $e_2^*(\alpha)$ it is 1%. The multipliers (10), with α instead of x , satisfy the stability conditions of section 2. The stability of the procedure means its convergence, which is also evident from the improvement of accuracy.

5. Critical screening

An important quantity characterizing the features of the Yukawa potential is the critical screening parameter, that is, such a value of the screening parameter $\alpha = \alpha_c$ above which there are no bound states. This critical parameter is defined by the condition $e(\alpha_c) = 0$. For each approximation $e_k(\alpha)$ for the ground-state energy there exists the corresponding critical parameter α_k given by the equation

$$e_k(\alpha_k) = 0. \quad (56)$$

From the approximations $e_k(\alpha)$ obtained in the previous section, we find the sequence of approximations for the critical screening parameters:

$$\alpha_1 = 1 \quad \alpha_2 = 1.0833. \quad (57)$$

To employ the self-similar renormalization for the sequence $\{\alpha_k\}$, as is described in section 2, we compose a sequence $\{\alpha_k(\lambda)\}$ of the partial sums

$$\alpha_k(\lambda) = \sum_{i=1}^k (\alpha_i - \alpha_{i-1}) \lambda^{p_i} \quad (58)$$

in which $k \geq 1$ and $\alpha_0(\lambda) \equiv 0$. As is clear from equation (58),

$$\alpha_k = \lim_{\lambda \rightarrow 1} \alpha_k(\lambda). \quad (59)$$

Then the sequence of approximations

$$\begin{aligned} \alpha_1(\lambda) &= \alpha_1 \lambda^{p_1} \\ \alpha_2(\lambda) &= \alpha_1 \lambda^{p_1} + (\alpha_2 - \alpha_1) \lambda^{p_2} \end{aligned}$$

can be renormalized in the way prescribed by section 2. First, we define the expansion function $\lambda(f)$ by the equation

$$\alpha_1(\lambda) = \alpha_1 \lambda^{p_1} = f$$

which gives

$$\lambda(f) = \left(\frac{f}{\alpha_1} \right)^{1/p_1}.$$

Writing the cascade velocity as

$$v_1(f) = \alpha_2(\lambda(f)) - \alpha_1(\lambda(f)) = (\alpha_2 - \alpha_1) \lambda^{p_2}(f)$$

we come to the evolution integral

$$\int_{\alpha_1(\lambda)}^{\alpha_2^*(\lambda)} \frac{df}{(\alpha_2 - \alpha_1) \lambda^{p_2}(f)} = t^*. \quad (60)$$

Notice that $\alpha_2^*(\lambda)$ in equation (60) also depends on the parameters

$$p \equiv p_1 \geq 0 \quad q \equiv \frac{p_2}{p_1} - 1 \geq 0 \quad (61)$$

so that we may write

$$\alpha_2^*(\lambda) = \alpha_2^*(\lambda, p, q). \quad (62)$$

Integrating equation (60), we obtain

$$\alpha_2^*(\lambda, p, q) = \left[\frac{\alpha_1^{1+q} \lambda^{pq}}{\alpha_1 - q(\alpha_2 - \alpha_1) \lambda^{pq} t^*} \right]^{1/q}. \quad (63)$$

To define p and q , consider the sequence $\{\bar{y}_k(f)\}$ of the terms $\bar{y}_k(f) \equiv \alpha_k(\lambda(f))$. Thus, we have

$$\begin{aligned}\bar{y}_1(f) &= f \\ \bar{y}_2(f) &= f + (\alpha_2 - \alpha_1) \left(\frac{f}{\alpha_1}\right)^{q+1}.\end{aligned}$$

For the latter sequence we can find the multipliers defined as in equation (14). As is obvious, $M_1 = 1$ and

$$M_2(\lambda, p, q) = 1 + (\alpha_2 - \alpha_1)(1 + q)\lambda^{pq}. \quad (64)$$

The values of p and q are chosen so as to satisfy the principle of maximal stability (15), with p and q playing the role of control functions. Since, according to condition (59), we must put at the end $\lambda \rightarrow 1$, we can consider the multiplier (64) for $\lambda \sim 1$. In the case when $\lambda > 1$, the minimum of $|M_2|$ from equation (64) is provided by $q = 0$. But if $\lambda < 0$, then this minimum can occur at $q = 1$. Here we keep in mind that q , given by equation (61), is an integer and that the difference $\alpha_2 - \alpha_1$ is positive in agreement with equation (57). In this way, from expression (63) we derive

$$\alpha_2^*(\lambda, p, 0) = \alpha_1 \lambda^p \exp\left(\frac{\alpha_2 - \alpha_1}{\alpha_1} t^*\right) \quad (65)$$

if $q = 0$, and

$$\alpha_2^*(\lambda, p, 1) = \frac{\alpha_1^2 \lambda^p}{\alpha_1 - (\alpha_2 - \alpha_1) \lambda^p t^*} \quad (66)$$

when $q = 1$.

The effective time t^* has the meaning of the minimal number of steps providing the renormalization of α_k , when $\lambda \rightarrow 1$. If we put $\lambda \rightarrow 1$ in the evolution integral (60) before the integration, then for α_2^* we get $\alpha_1 + (\alpha_2 - \alpha_1)t^*$. From here we see that $t^* = 0$ gives α_1 , one step, that is $t^* = 1$, leads to α_2 , and $t^* = 2$ results in $2\alpha_2 - \alpha_1$. Therefore, the minimal number of steps necessary for obtaining a non-trivial renormalization is $t^* = 2$.

Equations (65) and (66) show that, when $\lambda = 1$, then α_2^* does not depend on p . Consequently, we may write

$$\alpha_2^*(1, q) \equiv \alpha_2^*(1, p, q). \quad (67)$$

Putting $t^* = 2$ and $\lambda = 1$ in equations (65) and (66), we obtain

$$\alpha_2^*(1, 0) = \alpha_1 \exp\left(2 \frac{\alpha_2 - \alpha_1}{\alpha_1}\right) \quad (68)$$

and, respectively,

$$\alpha_2^*(1, 1) = \frac{\alpha_1^2}{3\alpha_1 - 2\alpha_2}. \quad (69)$$

As the final answer we set

$$\alpha_2^* = \frac{1}{2} [\alpha_2^*(1, 0) + \alpha_2(1, 1)]. \quad (70)$$

Substituting the numerical values from equation (57) into formulae (68) and (69), we have

$$\alpha_2^*(1, 0) = 1.1813 \quad \alpha_2^*(1, 1) = 1.1919.$$

Hence, equation (70) yields

$$\alpha_2^* = 1.1906.$$

This value of the critical screening parameter coincides with the result of numerical integration [11].

In conclusion, we have applied the self-similar renormalization theory [15–19] to calculating the energy and the critical screening parameter for the Schrödinger equation with the Yukawa potential. The calculated values are in good agreement with the results of the numerical computation. This demonstrates that renormalization-group techniques can be successfully employed to solve the Schrödinger equation, not only with simple anharmonic potentials [28, 29], but also for more realistic cases, such as the Yukawa potential that is often met in different physical problems. To obtain an accurate value of the critical screening parameter, we have used a method analogous to algebraic self-similar renormalization [30]. We have considered here mainly the ground-state level, although the procedure we have demonstrated is also applicable to excited levels, but calculations then become a little more cumbersome. We hope that the results we have obtained are sufficient for showing the usefulness of renormalization-group techniques in quantum mechanics.

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