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Nonperturbative approach to screened Coulomb potentials

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The energy levels of two simple examples of screened Coulomb potentials have been analyzed using nonperturbative methods. The analysis indicates that the energy levels as a function of the perturbation parameter λ have a branch cut along the negative real axis, starting from the origin. Furthermore, there are singularities on the second sheet, along $|\lambda| e^{\pm 3\pi i/2}$ for $|\lambda|\to 0$. As a consequence of these singularities, the energy levels have an asymptotic series in λ, which means that one cannot use a power series in λ to describe the energy levels to an arbitrary accuracy. The approximate but nonperturbative expression for the energy levels, which has been obtained by using dispersion relations, predicts energy levels which are in good agreement with those obtained from variational calculations.

I. INTRODUCTION

Most of the one-particle potentials that are encountered in quantum-mechanical applications do not allow closed exact solutions either for the energy eigenvalues or for the wave functions. In these cases, one resorts to approximate methods which may be suitable to the particular situation, to obtain approximate solutions. Perhaps the most useful solutions in this context are the perturbative solutions. This is due to the observation that in most of these problems, the Hamiltonian can be written as a sum of a major term which allows exact solutions and a "small" perturbing term. One may then obtain solutions in the form of perturbation series which agree with the exact solutions to an accuracy of increasing powers of the perturbation "parameters."

An important question which needs to be answered in determining the usefulness of a perturbation solution is whether a perturbation solution is meaningful in the situation: Specifically, does the perturbation series converge for any value of the perturbation parameter? If it does, what is the domain of convergence for the series? It is a very interesting situation that even though the formal series may diverge, if the series is asymptotic it can be quite useful for practical calculations. This may very likely be the actual situation for the perturbation expansions in quantum electrodynamics.[1]

Many of the problems faced by the perturbation approaches and their possible solutions are admirably illustrated by the anharmonic oscillator, which is described in the one-dimensional case by the Hamiltonian

$$H=(p^2/2m)+\tfrac{1}{2}kx^2+\lambda x^4 . \tag{1}$$

This Hamiltonian is of interest not only as a correction to the simple harmonic socillator which is a good approximation to many physical situations, but also because it describes the one-dimensional $\lambda\phi^4$ field theory without normal ordering. It was shown by Bender and Wu[2] that the energy levels of this Hamiltonian have a three-sheeted structure with $\lambda=0$ being the accumulation point of branch points on the lower sheets. The techniques used by Bender and Wu in proving this were approximate, but their results have since then been obtained from more rigorous analyses.[3,4] The perturbation series for the bound-state energy levels, in powers of λ is asymptotic in this case[5] so that for a given value of λ, there is an optimum number of terms in the series which gives the best approximation to the actual energy levels. It has also been pointed out that better approximations can be obtained by using Borel summations[6] for the series and by using Padé approximants.[7] Some of the other attempts at evaluation of anharmonic corrections have used Hill determinants[8] and nonpolynomial interactions.[9] All in all, one observes an impressive variety of techniques in the analysis of the anharmonic oscillator.

The problem of screened Coulomb potential is of great importance in all atomic phenomena involving electronic transitions. It has been analyzed numerically and analytically by several procedures such as the WKBJ method,[10] the quantum-defect method,[11] and different types of perturbation methods.[12] Of these, the perturbation approach directly provides systematic solutions as a series in powers of the perturbation parameter. Here, there have been significant developments[12] from the practical point of view of obtaining energy levels and wave functions within restricted regions inside the atoms. However there have not been corresponding attempts to determine the formal analytic structure of the energy levels and the wave functions as functions of the perturbation parameter, and hence the convergence properties of the perturbation series.

In this paper, we analyze the analyticity properties of the energy levels of the screened Coulomb potential for small values of the perturbation parameter. Specifically, we will consider two types of potentials. In the first part, we consider

$$V(r) = -z/r + \lambda r . \tag{2}$$

From the analogy with the anharmonic oscillator, one might expect that in this case also $\lambda = 0$ is a singular point and the perturbation series is asymptotic. We indeed find this to be the situation and obtain an approximate but nonperturbative expression for the energy levels for small values of λ, which illustrates these properties. The techniques used in this analysis are essentially those used by Bender and Wu[5] in their analysis of the anharmonic oscillator. In the second part we consider potentials of the form

$$V(r) = -\frac{z}{r} + \lambda \sum_{i=0}^{\infty} a_i (\lambda r)^i . \tag{3}$$

This type of potential has been used by Pratt and Tseng,[13] the understanding being that the screening effect is better represented by including more terms in the expansion. To study the properties of the resulting perturbation series in powers of λ, we analyze the energy levels for the representative potential

$$V(r) = -\frac{z}{r} + \lambda \frac{(z-1)}{1+\lambda r} \tag{4}$$

which describes screened Coulomb potential correctly for both $\lambda r \ll 1$ and $\lambda r \gg 1$. We obtain an approximate expression for the energy levels as a dispersion integral. We deduce that $\lambda = 0$ is again a branch-point singularity and very likely an accumulation point of singular points on the second sheet. The series in powers of λ is found to be asymptotic, which means that the perturbation series is not rigorously admissible. However, for a given value of λ, there is an optimum number of terms which could give a good approximation to the actual energy levels and which could be quite useful for practical calculations. Many of the results for this potential (4) are also valid for other potentials.

We discuss in a separate section the practical utility of the nonperturbative but approximate expression for the energy levels for the potential (4). The agreement of the values of the energy levels of the atoms predicted, with the experimentally observed values and with those obtained from variational calculations is very good, thus suggesting the usefulness of a nonperturbative though approximate approach to the problem of the screened Coulomb potential.

II. ENERGY LEVELS FOR PERTURBATION λr

The total Hamiltonian for this interaction is

$$H = p^2 - z/r + \lambda r , \tag{5}$$

where the mass is expressed in units of $2m$, m being the mass of the particle. Since the perturbation term λr dominates the interaction for $r \to \infty$, we expect the analytic properties of the energy levels to be similar to those of the anharmonic oscillator.[2] For the same reason, it admits an analysis similar to the one used for the anaharmonic oscillator. We first point out some general analyticity properties of the energy levels and then obtain a nonperturbative but approximate expression for the energy levels in the form of a dispersion integral.

A. Real positive λ

The asymptotic behavior of the wave functions is determined by the λr term in the interaction and for λ real and positive, it is given by

$$\psi(r) \underset{r\to\infty}{\simeq} \exp(-\tfrac{2}{3}\lambda^{1/2} r^{3/2}) . \tag{6}$$

Furthermore, one can take $\psi(r)$ to be real in this region. Then, for a change $\delta\lambda$ in λ, one has

$$\begin{aligned} &E(\lambda) \to E(\lambda) + \delta E(\lambda) , \\ &\psi(r,\lambda) \to \psi(r,\lambda) + \delta\psi(r,\lambda) , \end{aligned} \tag{7}$$

so that

$$H(\lambda)\delta\psi(r,\lambda) + \delta\lambda r \psi(r,\lambda) = \delta E(\lambda)\psi(r,\lambda) + E(\lambda)\delta\psi(r,\lambda) . \tag{8}$$

Multiply the two sides by $\psi(r,\lambda)$ and integrate by parts to obtain

$$\delta\lambda \langle \psi(\lambda) \,|\, r \,|\, \psi(\lambda) \rangle = \delta E(\lambda) \langle \psi(\lambda) \,|\, \psi(\lambda) \rangle , \tag{9}$$

where $|\psi(\lambda)\rangle$ is the state vector corresponding to the wave function $\psi(r,\lambda)$, or

$$\frac{\partial E(\lambda)}{\partial \lambda} = \frac{\langle \psi(\lambda) \,|\, r \,|\, \psi(\lambda) \rangle}{\langle \psi(\lambda) \,|\, \psi(\lambda) \rangle} . \tag{10}$$

Since the expression on the right exists and is finite in view of (6), $E(\lambda)$ is real and analytic for λ real and positive (i.e., $\lambda > 0$) in the sense that the first derivative exists.

B. The point $\lambda = 0$

We now show that $\lambda = 0$ must be a singular point. For this, we first subject our system to the

Symanzik scale transformation[3]:

$$p \to \alpha p\,, \quad r \to r/\alpha \tag{11}$$

for which the corresponding unitary transformation takes the Hamiltonian (5) into

$$H \to \alpha^2\left(p^2 - \frac{z/\alpha}{r} + \frac{\lambda r}{\alpha^3}\right). \tag{12}$$

With the choice $\alpha^3 = \lambda$, one has

$$H \to \lambda^{2/3}\left(p^2 - \frac{z\lambda^{-1/3}}{r} + r\right) \tag{13}$$

from which it follows that the energy levels satisfy the property

$$E(z,\lambda) = \lambda^{2/3}E(z\lambda^{-1/3}, 1)\,. \tag{14}$$

Suppose that $\lambda = 0$ is a nonsingular point. We start from large positive λ, move along the real axis towards zero, and after circling the origin go back to infinity. If $\lambda = 0$ is nonsingular, one then has from (14),

$$\begin{aligned}\lim_{\lambda\to\infty} E(Z,\lambda) &= \lambda^{2/3}E(0,1)\\ &= e^{4\pi i/3}\lambda^{2/3}E(0,1)\,,\end{aligned} \tag{15}$$

which is contradictory. Hence $\lambda = 0$ is a singular point of $E(z,\lambda)$.

C. Real negative λ

Here we consider the properties of the energy levels for $\lambda < 0$. We confine ourselves only to the S-wave and evaluate explicitly the imaginary part of the energy level $E_N(\lambda)$ for small, real and negative λ, by using the WKB method.[5]

The radial equation for the S-wave wave function is

$$\left(-\frac{d^2}{dr^2} - \frac{z}{r} + \lambda r\right)\chi(r) = E_N(\lambda)\chi(r) \tag{16}$$

with

$$\chi(r) = rR(r)\,, \tag{17}$$

where $R(r)$ is the radial wave function, and N is the total quantum number. The turning points for this problem are

$$r_1 = \frac{E_N}{2\lambda}\left[1 - \left(1 + \frac{4\lambda z}{E_N^2}\right)^{1/2}\right], \tag{18}$$

$$r_2 = \frac{E_N}{2\lambda}\left[1 + \left(1 + \frac{4\lambda z}{E_N^2}\right)^{1/2}\right], \tag{19}$$

which for small values of λ have the approximate expressions

$$r_1 \approx -z/E_N\,, \tag{20}$$

$$r_2 \approx E_N/\lambda + z/E_N\,. \tag{21}$$

(i) Region $r \sim r_1$: The equation to be solved is

$$\left(\frac{d^2}{dr^2} + \frac{z}{r} + E_N\right)\chi(r) = 0\,. \tag{22}$$

The solution which is regular at $r = 0$ is given by

$$\chi(r) = Are^{-\epsilon r}\,{}_1F_1(1 - z/2\epsilon\,, 2, 2\epsilon r)\,, \tag{23}$$

where

$$\epsilon = (-E_N)^{1/2} \tag{24}$$

and ${}_1F_1$ is the confluent hypergeometric function,

$${}_1F_1(a,b,x) = 1 + \frac{a}{b}\frac{x}{1!} + \frac{a(a+1)}{b(b+1)}\frac{x^2}{2!} + \cdots\,. \tag{25}$$

If we normalize $\chi(r)$ so as to give

$$4\pi\int_0^\infty [\chi(r)]^2\,dr = 1 \tag{26}$$

for the unperturbed value of $\epsilon = z/2N$, then

$$A = \frac{1}{(8\pi)^{1/2}}\left(\frac{z}{N}\right)^{3/2}. \tag{27}$$

The asymptotic behavior of $\chi(r)$ for

$$z/2\epsilon = N - \delta \tag{28}$$

where δ is infinitesimally small, is given by

$$\begin{aligned}\chi(r) \xrightarrow[r\to\infty]{} & A(-1)^{N-1}re^{-\epsilon r}\\ & \times[(2\epsilon r)^{N-1}/N! + (N-1)!\,\delta(2\epsilon r)^{-N-1}e^{2\epsilon r}]\,.\end{aligned} \tag{29}$$

(ii) Region from r_1 to r_2: In the region $r_1 \ll r$, $r_2 \gg r$, one can use the WKB solution to Eq. (16):

$$\begin{aligned}\chi_W(r) &= c_1 p^{-1/2}\exp\left(\int_{r_1}^{r} p\,dr\right)\\ &\quad + c_2 p^{-1/2}\exp\left(-\int_{r_1}^{r} p\,dr\right),\end{aligned} \tag{30}$$

where the subscript W indicates that we are using the WKB approximation, and

$$p = (\lambda r - z/r - E_N)^{1/2}\,. \tag{31}$$

For $r \gg r_1$ but $r \ll r_2$, one can evaluate the integrals in (30) approximately to obtain

$$\chi(r) \approx c_1\epsilon^{-1/2}\exp[I(r)] + c_2\epsilon^{-1/2}\exp[-I(r)]\,, \tag{32}$$

where

$$I(r) = \epsilon r - \frac{z}{2\epsilon}\ln r - \frac{z}{2\epsilon} - \frac{z}{\epsilon}\ln 2 + \frac{z}{2\epsilon}\ln\left(\frac{z}{\epsilon^2}\right). \tag{33}$$

Comparison of this with the asymptotic behavior (29) gives

$$c_1 = A(-1)^{N-1}(N-1)!\,\frac{e^N\delta}{zN^{N-1}}\,\epsilon^{1/2}\,, \tag{34}$$

$$c_2 = A(-1)^{N-1}\,\frac{N^{N+1}e^{-N}}{zN!}\,\epsilon^{1/2}\,, \tag{35}$$

to the leading order in δ.

We are now in a position to determine the imaginary part of $E_N(\lambda)$. For this we first note the relation

$$\mathrm{Im}E_N(\lambda) = \frac{J(r)}{\int_0^r \chi^*(r')\chi(r')\,dr'}\,, \tag{36}$$

where

$$J(r) = \frac{i}{2}\left(\chi^*(r)\frac{d}{dr}\chi(r) - \chi(r)\frac{d}{dr}\chi^*(r)\right). \tag{37}$$

This result is derived by multiplying (16) by $\chi^*(r)$, subtracting the complex conjugate of the result, and integrating by parts. The expression $J(r)$ is evaluated at $r > r_2$ by using the WKB approximation (30) and going around r_2 to avoid the difficulties with the turning point r_2. Using the continuation relations[5,14] for the turning point r_2, one has

$$J(r) = |c_2|^2\epsilon^{-1}\exp(-2I_{12})\,, \tag{38}$$

where

$$I_{12} = \int_{r_1}^{r_2} (\lambda r - z/r - E_N)^{1/2}\,dr\,. \tag{39}$$

For $\lambda \to 0$, this integral is found to be

$$I_{12} \approx -\frac{2\epsilon^3}{3\lambda} - \frac{z}{2\epsilon}\ln\left(-\frac{16\epsilon^4}{\lambda z}\right) - \frac{z}{2\epsilon}\,. \tag{40}$$

From the perturbative relation

$$\epsilon^2 \approx \frac{z^2}{4N^2} - \frac{3N^2}{z}\lambda \tag{41}$$

to terms linear in λ, use of which is justified by the result that $\epsilon(\lambda)$ has an asymptotic series as will be shown later, one obtains

$$I_{12} \approx -\frac{z^3}{12\lambda N^3} - N\ln\left(-\frac{z^3}{\lambda N^4}\right) + \frac{N}{2}\,. \tag{42}$$

The major contribution to the integral in the denominator of (36) comes from the small-r region. Thus to the leading order in λ, one has from (26), for $r > r_2$,

$$\int_0^r [\chi(r')]^2\,dr' = \frac{1}{4\pi}\,. \tag{43}$$

Combining the results (36), (38), (42), (43), (35), and (27), one finally gets

$$\mathrm{Im}\,E(\lambda) = \frac{z^3}{2N^3}\,\frac{N^{2N+2}e^{-2N}}{z^2(N!)^2} \times \exp\left[\frac{z^3}{6\lambda N^3} + 2N\ln\left(-\frac{z^3}{\lambda N^4}\right) - N\right] \tag{44}$$

for $\lambda < 0$ but small. This expression can also be written as

$$\mathrm{Im}E(\lambda) = g(N,z)(-\lambda)^{-2N}\exp(z^3/6\lambda N^3)\,, \tag{45}$$

where

$$g(N,z) = \frac{1}{2}\left(\frac{z}{N}\right)^{6N+1}\frac{e^{-3N}}{(N!)^2}\,. \tag{46}$$

D. Dispersion relations

From the above analysis, it follows that $E(\lambda)$ has a cut along the negative real axis. We assume that there are no other singularities on the first sheet, away from the real axis. Guided by the asymptotic behavior (15) for $E(\lambda)$, we write once-subtracted dispersion relations:

$$E_N(\lambda) = E_N(0) + \frac{\lambda}{\pi}\int_{-\infty}^0 \frac{\mathrm{Im}\,E_N(\lambda')}{\lambda'(\lambda'-\lambda)}\,d\lambda'\,. \tag{47}$$

Furthermore, one may write

$$E_N(\lambda) = E_N(0) + \sum_{k=1}^{\infty} A_N^k\lambda^k\,, \tag{48}$$

where

$$A_N^k = \frac{1}{\pi}\int_{-\infty}^0 \frac{\mathrm{Im}E_N(\lambda')}{(\lambda')^{k+1}}\,d\lambda'\,. \tag{49}$$

If one assumes that the major contribution to the dispersion integrals comes from the small-λ' region, we can use (45) to obtain

$$E_N(\lambda) = -\frac{z^2}{4N^2} + \frac{\lambda g(N,z)}{\pi} \times \int_{-\infty}^0 \frac{(-\lambda')^{-2N}\exp(z^3/6\lambda' N^3)}{\lambda'(\lambda'-\lambda)}\,d\lambda' \tag{50}$$

and

$$A_N^k = [g(N,z)/\pi](-1)^{k+1}(6N^3/z^3)^{2N+k}\,\Gamma(2N+k)\,. \tag{51}$$

This indicates that the series (48) is asymptotic. It is also possible to express (50) as a partial sum

$$E_N(\lambda) = -\frac{z^2}{4N^2} + \frac{g(N,z)}{\pi}\left[\sum_{k=1}^{n}(-1)^{k+1}\lambda^k\left(\frac{6N^3}{z^3}\right)^{2N+k}\Gamma(2N+k) + (-1)^n\left(\frac{6N^3}{z^2}\right)^{2N+n+1}\lambda^{n+1}\int_0^\infty \frac{x^{2N+n}e^{-x}}{1+6\lambda N^3x/z^3}\,dx\right]. \tag{52}$$

The integral in (52) is bounded by $\Gamma(2N+n+1)$ which again confirms that $E_N(\lambda)$ has an asymptotic series expansion. Of course this is an approximate expression for $E_N(\lambda)$ since one is using an $\mathrm{Im}E(\lambda')$, which is valid for small λ'. However the coefficients of higher powers of λ are expected to be more accurately represented since the small-λ' region is more important for them.

E. Continuation onto the second sheet

The integral (50) can be used for continuing $E_N(\lambda)$ onto the second sheet. As λ encircles the origin and goes onto the second sheet, we distort the path of integration. Because of the form of the integrand, the distortion for $\lambda \to 0$ is allowed only if $\text{Re}\,\lambda < 0$. This means that after encircling the origin, we come across singularities at

$$\arg\lambda = \pm \tfrac{3}{2}\pi . \tag{53}$$

This result is similar to the one for the anharmonic oscillator.[2,3,9]

III. ENERGY LEVELS FOR PERTURBATION $\lambda(z-1)/(1+\lambda r)$

The perturbation λr discussed in the last section can be regarded as representing a reasonable first-order correction to the Coulomb potential inside the atom. However, it differs violently from the expected screened Coulomb potential outside the atom. A perturbation which has the correct asymptotic behavior is given by the Hamiltonian

$$H = p^2 - \frac{z}{r} + \frac{(z-1)\lambda}{1+r\lambda} . \tag{54}$$

In terms of

$$\beta = 1/\lambda ,$$

this Hamiltonian can be rewritten as

$$H = p^2 - \frac{z}{r} + \frac{z-1}{r+\beta} . \tag{55}$$

We will first point out some general properties of the energy levels of this Hamiltonian and then obtain an approximate but nonperturbative expression for the energy levels as a dispersion integral.

A. Real positive β

For $\beta > 0$, the Hamiltonian H satisfies the inequality

$$H < p^2 - 1/r , \tag{56}$$

so that the energy levels satisfy the inequality

$$E_N(z,\beta) < E_N , \tag{57}$$

where E_N are the Coulomb energy levels with $z = 1$. It therefore follows that $E_N(z,\beta)$ is negative definite and real since H is Hermitian. One may also take $\psi(r)$ to be real. Then for a change $\delta\beta$ in β, one has

$$\begin{aligned} &E(\beta) \to E(\beta) + \delta E(\beta) , \\ &\psi(r,\beta) \to \psi(r,\beta) + \delta\psi(r,\beta) , \end{aligned} \tag{58}$$

so that

$$H(\beta)\delta\psi(r,\beta) - (z-1)\delta\beta \frac{1}{(r+\beta)^2}\psi(r,\beta) = \delta E(\beta)\psi(r,\beta) + E(\beta)\delta\psi(r,\beta) . \tag{59}$$

Multiplying the two sides by $\psi(r,\beta)$ and integrating by parts, one obtain

$$\frac{\partial E(\beta)}{\partial \beta} = -(z-1)\frac{\langle \psi(\beta) \,|\, (r+\beta)^{-2} \,|\, \psi(\beta)\rangle}{\langle \psi(\beta) \,|\, \psi(\beta)\rangle} . \tag{60}$$

Since the right-hand side exists and is finite, $E(\lambda)$ is real and analytic for $\beta > 0$ in the sense that the first derivative exists. It should also be noted that since $\partial E(\beta)/\partial\beta < 0$ and $E(\beta = 0)$ is the Coulomb energy level with $z = 1$, the relation (57) follows.

B. A lemma for $\beta < 0$

Here we derive an expression for $\text{Im}E(\beta + i\epsilon)$ for $\beta < 0$, in terms of the value of the wave function at $r = -\beta$. We begin with the general relation

$$\left(H_0 + \frac{z-1}{r+\beta+i\epsilon}\right)\psi(r,\beta+i\epsilon) = E(\beta+i\epsilon)\psi(r,\beta+i\epsilon) , \tag{61}$$

where

$$H_0 = p^2 - z/r . \tag{62}$$

This can also be written as

$$\left(H_0 + \frac{z-1}{r+\beta-i\epsilon} - 2\pi i(z-1)\delta(r+\beta)\right)\psi(r,\beta+i\epsilon) = E(\beta+i\epsilon)\psi(r,\beta+i\epsilon) . \tag{63}$$

Multiplying the two sides by $\psi^*(r,\beta+i\epsilon)$ and integrating by parts, one obtains

$$E(\beta+i\epsilon) - E^*(\beta+i\epsilon) = -8\pi^2 i(z-1)\beta^2 \,|\psi(r,\beta+i\epsilon)|^2_{r=-\beta} . \tag{64}$$

In obtaining this relation, we have thrown away the surface terms so that it is valid only if $\psi(r,\beta+i\epsilon)$ vanishes for $r \to \infty$. We have also assumed a normalization

$$4\pi\int_0^\infty |\psi(r,\beta+i\epsilon)|^2 r^2\,dr = 1 . \tag{65}$$

Under these conditions one then has

$$\text{Im}E(\beta+i\epsilon) = -4\pi^2(z-1)\beta^2 \,|\psi(r,\beta+i\epsilon)|^2_{r=-\beta} . \tag{66}$$

In the next section, we will use this relation to advantage.

C. $\text{Im}E(\beta)$ for $\beta < 0$

As before, we confine ourselves to the S wave, and to large values of β or equivalently, to small values of λ. If $\psi(r,\beta+i\epsilon) \to 0$ for $r \to \infty$, we only need to know $\psi(-\beta,\beta+i\epsilon)$ in order to be able to determine $\text{Im}E(\beta)$ by using (66).

The radial equation for the S-wave wave function is

$$\left(-\frac{d^2}{dr^2}-\frac{z}{r}+\frac{z-1}{r+\beta}\right)\chi(r)=E_N(\beta)\chi(r) \tag{67}$$

with

$$\chi(r)=rR(r) \tag{68}$$

as before. The turning points for this case are

$$r_1=-\frac{1+\beta E_N}{2E_N}\left[1-\left(1-\frac{4zE_N\beta}{(1+\beta E_N)^2}\right)^{1/2}\right], \tag{69}$$

$$r_2=-\frac{1+\beta E_N}{2E_N}\left[1+\left(1-\frac{4zE_N\beta}{(1+\beta E_N)^2}\right)^{1/2}\right], \tag{70}$$

which for large values of β have the approximate expressions

$$r_1\approx -z/E_N\ , \tag{71}$$

$$r_2\approx -\beta+(z-1)/E_N\ . \tag{72}$$

(i) Region $r\sim r_1$: The equation for this region is the same as in the previous case, i.e., Eq. (22), as also the solution (23) and its asymptotic behavior (29).

(ii) Region from r_1 to r_2: In the region $r_1\ll r$ and $r_2\gg r$, one may use the WKB solution to Eq. (67),

$$\chi_W(r)=C_1p^{-1/2}\exp\left(\int_{r_1}^{r}p\,dr\right)+C_2p^{-1/2}\exp\left(-\int_{r_1}^{r}p\,dr\right), \tag{73}$$

where

$$p=\left(\frac{z-1}{r+\beta}-\frac{z}{r}-E_N\right)^{1/2}. \tag{74}$$

For $r\gg r_1$ but $r\ll r_2$, one can evaluate the integrals in (73) approximately to obtain

$$\chi(r)\approx C_1\epsilon^{-1/2}\exp[I(r)]+C_2\epsilon^{-1/2}\exp[-I(r)]\ , \tag{75}$$

where as before $\epsilon=(-E_N)^{1/2}$ and

$$I(r)=\epsilon r-\frac{z}{2\epsilon}\ln r-\frac{z}{2\epsilon}-\frac{z}{\epsilon}\ln 2+\frac{z}{2\epsilon}\ln\left(\frac{z}{\epsilon^2}\right). \tag{76}$$

Comparison of this with the asymptotic behavior (29) gives

$$C_1=A(-1)^{N-1}(N-1)!\frac{e^N\delta}{zN^{N-1}}\epsilon^{1/2}, \tag{77}$$

$$C_2=A(-1)^{N-1}\frac{N^{N+1}e^{-N}}{zN!}\epsilon^{1/2} \tag{78}$$

to leading order in δ where

$$\delta=N-z/2\epsilon\ . \tag{79}$$

Similarly, for $r_2-r\gg r_1$ but $r\sim r_2$, one has

$$\chi(r)\approx C_1\epsilon^{-1/2}\exp[I(\rho)]+C_2\epsilon^{-1/2}\exp[-I(\rho)]\ , \tag{80}$$

where

$$\rho=r-r_2$$

and

$$I(\rho)=\epsilon\rho+\frac{z-1}{2\epsilon}\ln\rho+\frac{z-1}{2\epsilon}-\frac{z-1}{2\epsilon}\ln\left(-\frac{z-1}{4\epsilon^2}\right)+I_{12} \tag{81}$$

with

$$I_{12}=\int_{r_1}^{r_2}p\,dr\approx-\epsilon\beta-\frac{z}{2\epsilon}\ln\left(-\frac{\beta\epsilon^2}{z}\right)-\frac{z-1}{2\epsilon}\ln\left(-\frac{\beta\epsilon^2}{z-1}\right)-\frac{2z-1}{\epsilon}\ln 2-\frac{2z-1}{2\epsilon}\ . \tag{82}$$

Here, we have dropped terms of the order $1/\beta$. Simplification of the above expressions and retention of the terms to the leading order in δ, leads to

$$I(\rho)\approx\epsilon\rho+\frac{z-1}{2\epsilon}\ln\rho-\frac{\beta z}{2N}-\frac{N}{z}-N\ln\left(\frac{\beta^2 z}{N^2}\right)+\frac{N}{z}\ln(-\beta)\ , \tag{83}$$

where we have used the perturbative relation

$$\epsilon^2\approx\frac{z^2}{4N^2}-\frac{z-1}{\beta} \tag{84}$$

which is justified by the result that $E(\lambda)$ has an asymptotic series as will be shown later.

(iii) Region $r\sim r_2$: The equation to be solved is

$$\left(\frac{d^2}{dr^2}-\frac{z-1}{r+\beta}+E_N\right)\chi(r)=0\ . \tag{85}$$

This can be transformed into Whittaker's equation.[15] The solution which decreases exponentially for $r-r_2\gg r_1$ is Whittaker's function:

$$\chi(r)=B\rho e^{-\epsilon\rho}U[1+(z-1)/2\epsilon,2,2\epsilon\rho]\ , \tag{86}$$

where B is the normalization constant, $\rho=r+\beta$, and

$$U(a,2,x)=\frac{1}{\Gamma(a-1)}\left({}_1F_1(a,2,x)\ln x+\sum_{r=0}^{\infty}\frac{a_r x^r}{(2)_r r!}\times[\psi(a+r)-\psi(1+r)-\psi(2+r)]\right)+\frac{1}{\Gamma(a)x}\ ,$$

$$a_r=a(a+1)\cdots(a+r-1),\quad a_0=1\ , \tag{87}$$

$$\psi(a)=\Gamma'(a)/\Gamma(a)\ .$$

For determining the normalization constant B, we look at the behavior of $\chi(r)$ for $r-r_2 \ll r_1$ but $r\sim r_2$:

$$\chi(r) \xrightarrow[\rho\to-\infty]{} B(2\epsilon)^{-1-(z-1)/2\epsilon}\rho^{-(z-1)/2\epsilon}e^{-\epsilon\rho}. \quad (88)$$

Comparing this with the second term in the asymptotic behavior (80) of the WKB solution, we obtain

$$B = A\,\frac{(-1)^{N-1}}{N!}\left(-\frac{\beta z}{N}\right)^{N(2-1/z)}\exp\left(\frac{\beta z}{2N}-\frac{N(z-1)}{z}\right), \quad (89)$$

where A is given by (27).

We are now in a position to evaluate the $\mathrm{Im}E(\beta)$ by using (66). Since the leading contribution to the normalization integral (65) comes from the small-r region, one can take the wave function (23) for normalizing the wave function. Since this wave function satisfies the condition (26), our wave functions are normalized according to the requirement of the relation (66). Therefore using (86), (87), and (88) we have

$$\mathrm{Im}E_N(\beta+i\epsilon) = -4\pi^2(z-1)\,\frac{|B|^2}{[2\epsilon\Gamma(1+(z-1)/2\epsilon)]^2}\;. \quad (90)$$

This can also be written in the form

$$\mathrm{Im}E_N(\beta+i\epsilon) = -f(N,z)(-\beta)^{2(2z-1)N/z}\exp(\beta z/N), \quad (91)$$

where

$$f(N,z) = \frac{\pi z^3}{2(z-1)N^3}\left(\frac{z}{N}\right)^{2(2z-1)N/z} \times \frac{\exp[-2N(z-1)/z]}{(N!)^2[\Gamma((z-1)N/z)]^2}\;. \quad (92)$$

D. Dispersion relation

The preceding analysis indicates that $E_N(\lambda)$ has a cut along the negative real axis. Furthermore, for $\lambda\to\infty$, the energy levels are expected to tend to those of Coulomb potential with $z=1$. Hence, with the assumption that there are no other singularities on the first sheet away from the real axis, one may write once-subtracted dispersion relations for $E_N(\lambda)$:

$$E_N(\lambda) = E_N(0) + \frac{\lambda}{\pi}\int_{-\infty}^{0}\frac{\mathrm{Im}E_N(\lambda'+i\epsilon)}{\lambda'(\lambda'-\lambda)}\,d\lambda'\;. \quad (93)$$

Furthermore, if one writes

$$E_N(\lambda) = E_N(0) + \sum_{k=1}^{\infty} A_N^k\lambda^k\;, \quad (94)$$

we have

$$A_N^k = \frac{1}{\pi}\int_{-\infty}^{0}\frac{\mathrm{Im}E_N(\lambda'+i\epsilon)}{(\lambda')^{k+1}}\,d\lambda'\;. \quad (95)$$

If one assumes that the major contribution to the dispersion integrals comes from the small-λ' region, we can use (91) to obtain

$$E_N(\lambda) = -\frac{z^2}{4N^2} + \frac{\lambda f(N,z)}{\pi}\int_{-\infty}^{0}\frac{(-\lambda')^{2(1-2z)N/z}\exp(z/\lambda' N)}{\lambda'(\lambda'-\lambda)}\,d\lambda' \quad (96)$$

and

$$A_N^k = \frac{f(N,z)}{\pi}(-1)^{k+1}\left(\frac{N}{z}\right)^{k+2N(2z-1)/z}\Gamma(k+2N(2z-1)/z)\;, \quad (97)$$

which indicates that the series (94) is asymptotic. In using (91) it must be remembered that the phase of λ is opposite to that of β. It is also possible to express (96) as a partial sum

$$E_N(\lambda) = -\frac{z^2}{4N^2} + \frac{f(N,z)}{\pi}\Bigg[\sum_{k=1}^{n}\lambda^k(-1)^{k+1}\left(\frac{N}{z}\right)^{k+2N(2z-1)/z}\Gamma(k+2N(2z-1)/z) + (-1)^n\left(\frac{N}{z}\right)^{n+1+2N(2z-1)/z}\lambda^{n+1}\int_0^{\infty}\frac{x^{n+2N(2z-1)/z}e^{-x}}{1+\lambda Nx/z}\Bigg]dx\;. \quad (98)$$

The integral here is bounded by $\Gamma(n+1+2N(2z-1)/z)$ for $\lambda>0$, which again confirms that $E_N(\lambda)$ has an asymptotic series expansion. The use of (96) which is valid for small λ' introduces an approximation in the above results, but the coefficients of higher powers of λ are expected to be given fairly accurately since the small-λ' region is more important for them.

E. Continuation to the second sheet

The integral (96) can be used for continuing $E_N(\lambda)$ onto the second sheet by distorting the path of integration. Because of the form of the integrand, the distortion for $\lambda\to 0$ is allowed only if $\mathrm{Re}\lambda<0$. This means that after encircling the origin, we come across singularities at

$$\arg\lambda = \pm\tfrac{3}{2}\pi \tag{99}$$

which is similar to the result (53) for the λr perturbation.

IV. COMPARISON WITH THE EXPERIMENTAL AND VARIATIONAL ENERGY LEVELS

We have shown in the previous sections that the energy levels for two "reasonable" screened potentials, i.e., potentials (2) and (4), have asymptotic series expansions. This is also expected to be true for potentials of the type

$$V(r) = -z/r + \lambda r^n e^{-\lambda r^m} \tag{100}$$

since for $\lambda < 0$, the energy levels will develop an imaginary part. For the energy levels with asymptotic series expansions, one cannot use perturbation series expansions to obtain the energy levels to an arbitrary accuracy. However the use of the first few terms may give fairly accurate values for the energy levels so that the perturbation series can yet be of some use.

In this section, we will consider the practical utility of the approximate but nonperturbative expansion for the energy levels $E_N(\lambda)$ for representative potential (54) of Sec. III. This is relevant in view of the above discussion that the perturbation series is expected to be asymptotic. Actually we will use twice-subtracted dispersion relations:

$$E_N(\lambda) = -\frac{z^2}{4N^2} + (z-1)\lambda + \frac{\lambda^2}{\pi}\int_{-\infty}^{0} \frac{\mathrm{Im}E_N(\lambda'+i\epsilon)}{\lambda'^2(\lambda'-\lambda)}\,d\lambda' , \tag{101}$$

with $\mathrm{Im}E_N(\lambda'+i\epsilon)$ given by (91) except for the sign. The reason for this is that we have already used the first two terms of (101) in obtaining (91). Furthermore, in the evaluation of $\mathrm{Im}E_N(\lambda'+i\epsilon)$ we have used WKB analysis in the region of r which satisfies $r_2 \gg r \gg r_1$ which is justified only if $r_2 > r_1$. From the approximate expressions (71) and (72), it therefore follows that the $\mathrm{Im}E_N(\lambda')$ given by (91) is valid only in the region

$$-\lambda' < z/8N^2 , \tag{102}$$

where we have neglected 1 compared to z. For our phenomenological analysis, therefore, we use

$$E_N(\lambda) = -\frac{z^2}{4N^2} + (z-1)\lambda + \frac{\lambda^2}{\pi}\int_{-z/8N^2}^{0} \frac{\mathrm{Im}E_N(\lambda'+i\epsilon)}{\lambda'^2(\lambda'-\lambda)}\,d\lambda' . \tag{103}$$

For determining λ we use the relation

$$\lambda = \lambda_0 z^{1/3} \tag{104}$$

corresponding to the z dependence of the reciprocal of the Thomas-Fermi radius of the atom.[12] We fit the experimental values[16] of the energy levels with $N=1,2$ for $z=14$ to $z=84$. The integration in (103) is carried out numerically, and we find that very good fits are obtained for a value of $\lambda_0 = 0.49$ in the units defined before, for which the Bohr radius a_0 has a value of 2, i.e., $\lambda_0 = 0.98/a_0$. The values of the energy levels E_1 and E_2 predicted are shown in Table I for z ranging from 14 to 84, at intervals of 5. The table also includes the experimentally observed energy levels[16] and those obtained from variational calculations using Coulomb wave functions. Except for E_2 with $z=14$, the agreement between predictions and the experimental values as well as those from variational

TABLE I. Predicted and experimental binding energies E_N (in keV) with $N=1,2$ for some values of z.

z	Dispersion	E_1 Expt.	Variational	Dispersion	E_2 Expt.	Variational
14	−1.89	−1.84	−1.94	−9.17(−2)	−1.49(−1)	−1.61(−1)
19	−3.71	−3.61	−3.77	−3.42(−1)	−3.77(−1)	−3.94(−1)
24	−6.16	−5.99	−6.20	−7.24(−1)	−6.95(−1)	−7.45(−1)
29	−9.26	−8.98	−9.28	−1.24	−1.10	−1.22
34	−1.30(1)	−1.27(1)	−1.31(1)	−1.89	−1.65	−1.82
39	−1.74(1)	−1.70(1)	−1.74(1)	−2.70	−2.37	−2.59
44	−2.25(1)	−2.21(1)	−2.25(1)	−3.64	−3.22	−3.44
49	−2.82(1)	−2.79(1)	−2.83(1)	−4.73	−4.24	−4.50
54	−3.45(1)	−3.46(1)	−3.46(1)	−5.97	−5.45	−5.67
59	−4.15(1)	−4.20(1)	−4.16(1)	−7.35	−6.83	−7.01
64	−4.92(1)	−5.02(1)	−4.94(1)	−8.89	−8.38	−8.46
69	−5.76(1)	−5.94(1)	−5.77(1)	−1.06(1)	−1.01(1)	−1.01(1)
74	−6.66(1)	−6.95(1)	−6.66(1)	−1.24(1)	−1.21(1)	−1.18(1)
79	−7.63(1)	−8.07(1)	−7.63(1)	−1.44(1)	−1.43(1)	−1.38(1)
84	−8.66(1)	−9.31(1)	−8.66(1)	−1.65(1)	−1.69(1)	−1.58(1)

calculations is very satisfactory. The energy levels for higher N values or smaller z values should not be expected to come out correctly, in view of the fact that we have not taken into account the large-λ' contribution to the dispersion integral. This suggests that the nonperturbative approach to the screened Coulomb potential may be pertinent and useful from a practical point of view.

V. SUMMARY

We have analyzed the energy levels of two simple examples of screened Coulomb potentials by nonperturbative methods. We find that the energy levels as functions of the perturbation parameter λ, have a branch cut along the negative real axis, starting from the origin. Furthermore, there are singularities on the second sheet, for $\lambda \to 0$ with a phase of $\pm \frac{3}{2}\pi$, which prevent analytic continuation across $|\lambda| e^{\pm 3\pi i/2}$ and $|\lambda| \to 0$. The consequence of these singularities is that the energy levels have an asymptotic series in λ. Such a series is divergent, but for a given value of λ, the first few terms of the series can give a good approximation to the energy levels. The series may be useful to arbitrary accuracy if one uses Padé approximants[7] or Borel summations.[6]

The approximate but nonperturbative expression for the energy levels, which we have obtained by using dispersion relations and the WKB approximation to connect the known solutions in two separated regions, is found to predict the observed energy levels quite satisfactorily. This indicates that apart from the formal requirements, such nonperturbative analyses may have an important practical role in the description of screened Coulomb potentials.

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