

Home Search Collections Journals About Contact us My IOPscience

An improved calculation for screened Coulomb potentials in Rayleigh-Schrodinger perturbation theory

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 1985 J. Phys. A: Math. Gen. 18 1379 (http://iopscience.iop.org/0305-4470/18/9/020) View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 129.252.86.83 The article was downloaded on 31/05/2010 at 09:52

Please note that terms and conditions apply.

An improved calculation for screened Coulomb potentials in Rayleigh–Schrödinger perturbation theory

R Dutt[†], K Chowdhury[†] and Y P Varshni[‡]

⁺ Department of Physics, University of Visva-Bharati, Santiniketan-731235, West Bengal, India

‡ Department of Physics, University of Ottawa, Ottawa, Canada K1N 6N5

Received 6 November 1984

Abstract. Earlier works on screened Coulomb potentials using Rayleigh-Schrödinger perturbation theory have been re-examined. Instead of working with the usual Hulthén potential as the unperturbed Hamiltonian, we propose that a scaled Hulthén potential with modified strength and screening coefficient represents the lowest-order approximation for the static-screened Coulomb and exponential cosine-screened Coulomb potentials. The scale parameter appearing in the new Hulthén potential is then determined from the notion of the virial theorem and intuitive physical arguments. It is found that the accuracy of the predicted energy eigenvalues for the bound s states improves significantly even when the screening parameter is large and quite close to its critical value for which the quantum state becomes just bound. In spite of the simplicity of our approach, the numerical results compare fairly well with those obtained from rigorous analytic approximation methods.

1. Introduction

The problem of accurately determining the properties of the energy eigenvalues of spherically-symmetric-screened Coulomb potentials has been of considerable interest in numerous areas of physics for many years. Typical examples of this class of potentials are the well-known Yukawa or the static-screened Coulomb potential (SSCP)

$$V^{\rm SSCP}(r) = -\exp(-\lambda r)/r \tag{1.1}$$

and the exponential cosine screened Coulomb (ECSC) potential

$$V^{\text{ECSC}}(r) = -\exp(-\lambda r) \cos(\lambda r)/r$$
(1.2)

which have received wide applications in plasma physics (Margenau and Lewis 1959, Harris 1962), nuclear physics (Yukawa 1935, Green 1949) and solid state physics (Bonch-Bruevich and Glasko 1959, Hall 1962, Krieger 1969). Such potentials have been studied using many techniques, both numerical and analytical. The most widely investigated analytic approximation methods involve perturbative (Iafrate and Mendelsohn 1969, Lam and Varshni 1971, 1972, McEnnan *et al* 1976, Killingbeck and Galicia 1980, Lai 1981, 1982), variational (Lam and Varshni 1971, 1972, Roussel and O'Connell 1974) and non-perturbative techniques (Ecker and Weizel 1956, Lam and Varshni 1976, Mehta and Patil 1978, Ray and Ray 1980, Dutt *et al* 1981, Patil 1984, Gerry and Laub 1984).

The analytic methods in general have the common feature that the numerical accuracy of the predicted bound-state energies decreases rapidly as the screening

0305-4470/85/091379+10\$02.25 © 1985 The Institute of Physics

parameter λ approaches its critical value λ_c for which the state in question is just bound. In a perturbative approach, Lai (1981, 1982) obtained very accurate energy eigenvalues in the critical screening region ($\lambda/\lambda_c \approx 0.8$) both for the ssCP and the ECSC potential. He applied the Padé approximant technique to the analytic perturbation series obtained through the use of hypervirial and Hellman-Feynman theorems. Accurate energy eigenvalues have also been obtained in the framework of the 1/N expansion technique (Moreno and Zepeda 1984, Imbo *et al* 1984). Recently, Patil (1984) has proposed a non-perturbative method for obtaining very accurate energy eigenvalues for any nl state of the ssCP.

It has been observed that all these analytic methods, perturbative or non-perturbative, which give consistently good results for the bound-state energies for a wide range of the screening parameter, not only involve elaborate and rigorous analytic calculations but also require considerable computations for each numerical prediction. Furthermore, compact analytic expressions for the bound-state energies are not obtained in general.

In view of this, it is tempting as well as realistic to invoke a simple analytic approach without sacrificing the numerical accuracy which has hitherto been achieved in sophisticated analytic techniques. In this paper, we try to demonstrate that the traditional Rayleigh-Schrödinger (RS) perturbation method can lead to analytical approximations of the energies with a fairly good accuracy provided one makes the judicial choice for the unperturbed Hamiltonian. In earlier works, Lam and Varshni (1971, 1972) used the standard Hulthén potential

$$V_{\rm H}(r) = -\lambda \, \exp(-\lambda r) / [1 - \exp(-\lambda r)] \tag{1.3}$$

as the unperturbed potential for both the sSCP and the ECSC potential. Working with this prescription, although reasonable energy eigenvalues are obtained for small λ , there is wide discrepancy between the predicted energy eigenvalues and those found numerically from direct integration of the Schrödinger equation for a large screening parameter. For example, the Hulthén perturbation gives the wrong signature for the ground-state energy eigenvalue of the sSCP for $\lambda = 1$. This leads us to suspect that perhaps the screened Coulomb potentials of the form in (1.1) and (1.2) are not adequately described by the conventional form of the Hulthén potential in (1.3), particularly when λ is large and close to its critical value λ_c . We then conjecture that the screened Coulomb potentials may be better approximated by a scaled Hulthén potential

$$V_{\rm SH}(r) = -(a\lambda) \exp(-a\lambda r) / [1 - \exp(-a\lambda r)]$$
(1.4)

in which the coupling strength as well as the screening coefficient have been scaled up by the factor a which is greater than unity. Although it seems at the beginning that the scale parameter has been introduced in an *ad hoc* manner, we give reasons to determine it approximately using the virial theorem (Davydov 1976) and intuitive physical arguments. The value of a thus determined is found to be different for each screened potential. One of the interesting features of this approach is that even the rough estimate for the scale parameter gives substantial enhancement in the numerical accuracy of the predicted energy levels.

In § 2, we present the perturbative results up to first order using the scaled Hulthén potential as the unperturbed Hamiltonian. A compact analytic expression for the energy level for an arbitrary bound s state has been obtained from which the results for the sscp and ecsc potential can be reproduced separately by proper choice of the

variables involved. The prescription for determining the scale parameter is discussed in § 3. In § 4, our numerical results for the bound-state energies of 1s-4s states for both the ssCP and ECSC potential for various screening parameters are given and compared to those obtained from other analytic methods. For the sake of assessing the accuracy of our predicted results, we also tabulate the exact values obtained numerically (Rogers *et al* 1970) for the ssCP. As will be seen, our calculations for the energy levels are superior to the previous RS perturbation calculation of Lam and Varshni. It is very encouraging to note that our approach, although very simple, predicts results which are accurate within 2% for the screening parameter λ as large as $0.8\lambda_c$. The significance of our results is finally discussed and a few remarks are made in support of the present point of view.

2. RS perturbation method with the scaled Hulthén potential

For a unified treatment of the sSCP and the ECSC potential, we perform the calculation for the screened Coulomb potential

$$V_{\rm sc}(r) = -\exp(-\lambda r)\cos(\delta r)/r \tag{2.1}$$

which corresponds to the standard sSCP and ECSC forms in (1.1) and (1.2) for $\delta = 0$ and $\delta = \lambda$ respectively.

For perturbative calculation, we decompose the potential in (2.1) as the scaled Hulthén potential plus a perturbation H':

$$V_{\rm sc}(r) = -(a\lambda) \exp(-a\lambda r) / [1 - \exp(-a\lambda r)] + H'$$
(2.2)

where

$$H' = (a\lambda) \exp(-a\lambda r) / \{ [1 - \exp(-a\lambda r)] - \exp(-\lambda r) \cos(\delta r) / r \}.$$
(2.3)

The radial Schrödinger equation for l = 0 for the unperturbed potential may be written in atomic units ($\hbar = m = e = 1$)

$$d^{2}\chi_{n}(r)/dr^{2}+2\{E+(a\lambda)\exp(-a\lambda r)/[1-\exp(-a\lambda r)]\}\chi_{n}(r)=0$$
(2.4)

where $\chi_n(r) = rR_n(r)$.

.....

Equation (2.4) is exactly solvable and one obtains the following unperturbed energy eigenvalues and normalised eigenfunctions

$$E_{ns}^{(0)} = -\frac{1}{2} [(1/n) - (an\lambda/2)]^2$$
(2.5*a*)

$$\chi_{nS}^{(0)}(r) = \left(\frac{a\lambda(\beta_n - 1)(\beta_n + 2n - 1)}{2(\beta_n + n - 1)}\right)^{1/2} \exp(-\alpha_n a\lambda r)$$
$$\times \sum_{\nu=1}^n (-1)^{\nu-1} \binom{n-1}{\nu-1} \binom{n+\beta_n+\nu-2}{\nu} [1 - \exp(-a\lambda r)]^{\nu}$$
(2.5b)

in which

$$\alpha_n = (1/na\lambda) - (n/2)$$

$$\beta_n = (2/na\lambda) - n + 1.$$
(2.6)

Using the explicit expressions for the unperturbed energy eigenfunctions and eigenvalues, the first-order correction to the energy levels of the screened Coulomb potential $V_{\rm sc}(r)$ may be computed analytically. Using standard integrals (Gradshteyn and Ryzhik 1965) we then obtain

$$\Delta E_{ns}^{(1)} = \langle \chi_{ns}^{(0)} | H' | \chi_{ns}^{(0)} \rangle$$

$$= \frac{a\lambda (\beta_n - 1)(\beta_n + 2n - 1)}{2(\beta_n + n - 1)} \sum_{\mu=1}^{n} \sum_{\nu=1}^{n} (-1)^{\mu+\nu-2} {n-1 \choose \mu-1} {n-1 \choose \nu-1}$$

$$\times {n+\beta_n + \mu - 2 \choose \mu} {n+\beta_n + \nu - 2 \choose \nu} \left\{ \frac{\Gamma(2\alpha_n + 1)\Gamma(\mu + \nu)}{\Gamma(\mu + \nu + 2\alpha_n + 1)} + \frac{1}{2} (-1)^{\mu+\nu+1} \sum_{k=0}^{\mu+\nu} (-1)^{k+1} {\mu+\nu \choose k} \right\}$$

$$\times \log \left[\left(2\alpha_n + \frac{1}{a} + \mu + \nu - k \right)^2 + \frac{\delta^2}{\lambda^2 a^2} \right] \right\}.$$
(2.7)

Thus the binding energy for any bound s state may be obtained by combining the contributions of (2.5a) and (2.7). For numerical computations, we present here the explicit forms for the first four energy levels:

$$E_{1s} = \frac{(4-a^{2}\lambda^{2})}{8} - \frac{(4-a^{2}\lambda^{2})}{a^{2}\lambda^{2}} \{ \log[(1+\frac{1}{2}\lambda)^{2}+\frac{1}{4}\delta^{2}] - \frac{1}{2}\log[(1+\frac{1}{2}\lambda-\frac{1}{2}a\lambda)^{2}+\frac{1}{4}\delta^{2}] \}$$
(2.8)

$$E_{2s} = \frac{(1-4a^{2}\lambda^{2})}{8} - \frac{(1-4a^{2}\lambda^{2})}{16a^{4}\lambda^{4}} \{ -(1-a\lambda)^{2}\log[(1+\lambda-2a\lambda)^{2}+\delta^{2}] + 4(1-a\lambda)\log[(1+\lambda-a\lambda)^{2}+\delta^{2}] - 2(3-a^{2}\lambda^{2})\log[(1+\lambda)^{2}+\delta^{2}] + 4(1+a\lambda)\log[(1+\lambda+a\lambda)^{2}+\delta^{2}] - (1+a\lambda)^{2}\log[(1+\lambda+2a\lambda)^{2}+\delta^{2}] \}$$
(2.9)

$$E_{3s} = \frac{(4-81a^{2}\lambda^{2})}{72} - \frac{(4-81a^{2}\lambda^{2})}{39\,366a^{6}\lambda^{6}} \{-(1-3a\lambda)^{2}(2-3a\lambda)^{2} \\ \times \log[(2+3\lambda-9a\lambda)^{2}+9\delta^{2}] + 6(1-3a\lambda)(2-3a\lambda)^{2} \\ \times \log[(2+3\lambda-6a\lambda)^{2}+9\delta^{2}] - 3(2-3a\lambda)(10-15a\lambda-18a^{2}\lambda^{2}) \\ \times \log[(2+3\lambda-3a\lambda)^{2}+9\delta^{2}] + 2(4-9a^{2}\lambda^{2})(10-9a^{2}\lambda^{2}) \\ \times \log[(2+3\lambda)^{2}+9\delta^{2}] - 3(2+3a\lambda)(10+15a\lambda-18a^{2}\lambda^{2}) \\ \times \log[(2+3\lambda+3a\lambda)^{2}+9\delta^{2}] + 6(1+3a\lambda)(2+3a\lambda)^{2} \\ \times \log[(2+3\lambda+6a\lambda)^{2}+9\delta^{2}] - (1+3a\lambda)^{2}(2+3a\lambda)^{2} \\ \times \log[(2+3\lambda+9a\lambda)^{2}+9\delta^{2}] \}$$
(2.10)

$$E_{4s} = \frac{(1-64a^{2}\lambda^{2})}{32} - \frac{(1-64a^{2}\lambda^{2})}{1179\,648a^{8}\lambda^{8}} \\ \times \{-(1-2a\lambda)^{2}(1-4a\lambda)^{2}(1-6a\lambda)^{2} \\ \times \log[(1+2\lambda-8a\lambda)^{2}+4\delta^{2}] + 8(1-2a\lambda)^{2}(1-4a\lambda)^{2}(1-6a\lambda) \\ \times \log[(1+2\lambda-6a\lambda)^{2}+4\delta^{2}] - 4(1-2a\lambda)^{2}(1-4a\lambda)(7-28a\lambda-36a^{2}\lambda^{2})$$

$$\times \log[(1+2\lambda-4a\lambda)^{2}+4\delta^{2}]+8(1-4a\lambda)(1-4a^{2}\lambda^{2})(7-14a\lambda-24a^{2}\lambda^{2})$$

$$\times \log[(1+2\lambda-2a\lambda)^{2}+4\delta^{2}]-2(1-4a^{2}\lambda^{2})(35-380a^{2}\lambda^{2}+576a^{4}\lambda^{4})$$

$$\times \log[(1+2\lambda)^{2}+4\delta^{2}]+8(1+4a\lambda)(1-4a^{2}\lambda^{2})(7+14a\lambda-24a^{2}\lambda^{2})$$

$$\times \log[(1+2\lambda+2a\lambda)^{2}+4\delta^{2}]-4(1+2a\lambda)^{2}(1+4a\lambda)(7+28a\lambda-36a^{2}\lambda^{2})$$

$$\times \log[(1+2\lambda+4a\lambda)^{2}+4\delta^{2}]+8(1+2a\lambda)^{2}(1+4a\lambda)^{2}(1+6a\lambda)$$

$$\times \log[(1+2\lambda+6a\lambda)^{2}+4\delta^{2}]-(1+2a\lambda)^{2}(1+4a\lambda)^{2}(1+6a\lambda)^{2}$$

$$\times \log[(1+2\lambda+8a\lambda)^{2}+4\delta^{2}]-(1+2a\lambda)^{2}(1+4a\lambda)^{2}(1+6a\lambda)^{2}$$

(2.11)

The expressions in equations (2.8)-(2.11) are quite general in a sense that one obtains the results for the SSCP and ECSC potential just by setting $\delta = 0$ and $\delta = \lambda$ respectively. Furthermore, the analytic forms obtained by Lam and Varshni may be easily restored by using a = 1, $\delta = 0$ for the SSCP and a = 1, $\delta = \lambda$ for the ECSC potential.

For numerical work, it is now necessary to set the value of the scale parameter a which as yet remains arbitrary. Although there is no first principle to determine it uniquely, it will be shown that a rough estimate for it can be made following intuitive physical ideas.

3. Determination of the scale parameter

The scale factor can be determined in an approximate way from the behaviour of the energy eigenvalues in the neighbourhood of critical screening. When $\lambda = \lambda_c$, E = 0 and consequently the average kinetic energy is given by

$$\langle T \rangle = -\langle V \rangle. \tag{3.1}$$

It also follows from the standard virial theorem that

$$2\langle T \rangle = \langle r \, \mathrm{d} V / \mathrm{d} r \rangle \rangle. \tag{3.2}$$

Combining equations (3.1) and (3.2) gives

$$\langle V \rangle_{\lambda = \lambda_{c}} = -\frac{1}{2} \langle r \, \mathrm{d} \, V / \mathrm{d} \, r \rangle_{\lambda = \lambda_{c}}$$
(3.3)

Using either the sscP or the ECSC potential in equation (3.3), we find that one possible solution may be

$$\lambda_c r \simeq 1. \tag{3.4}$$

It is reasonable to assume that if accurate energy eigenvalues are to be obtained from the scaled Hulthén potential for $\lambda \approx \lambda_c$, the true potential and the approximate one should be fairly close to each other. We then require that the actual potential and the scaled Hulthén potential match with each other at $\lambda = \lambda_c$.

For the SSCP, we obtain

$$-\exp(\lambda_{\rm c} r)/r \simeq -(a\lambda_{\rm c})\exp(-a\lambda_{\rm c} r)/[1-\exp(-a\lambda_{\rm c} r)].$$
(3.5)

Equations (3.4) and (3.5) then give

$$e^{-a}(ea+1) - 1 = 0 \tag{3.6}$$

where $e = 2.718\ 282$. Solving equation (3.6) gives the effective scale factor for the sscp

$$a \simeq 1.75.$$
 (3.7)

Similar matching may also be done for the ECSC potential and we get a different scale factor

$$a \simeq 2.3. \tag{3.8}$$

Although we have made a crude estimation for the effective scale parameter, it turns out to be substantially different from a = 1 which corresponds to the simple Hulthén potential. Before proceeding further for numerical calculations, it is therefore necessary to convince ourselves about the proximity of the unperturbed potential and the actual screened Coulomb potential. For this purpose, the variation of the screened Coulomb potentials with the radial coordinate are shown in figure 1 along with the corresponding variations of the Hulthén and the scaled Hulthén potentials. It is remarkable that the scaled Hulthén potentials with a = 1.75 and a = 2.3 are in close agreement with the ssCP and the ECSC potential respectively, in contrast to the wide difference between the normal Hulthén potential and the screened Coulomb potential in the larger r region. This observation supports our conjecture that the scaled Hulthén potential should be a better choice than the conventional Hulthén potential as the lowest order approximation for a screened potential with 1/r singularity at the origin.



Figure 1. Product of rV(r) as a function of r for (a) the Hulthén potential, the scaled Hulthén potential with a = 1.75 and the ssCP for $\lambda = 0.4$ and (b) the Hulthén potential, the scaled Hulthén potential with a = 2.3 and the ECSC potential for $\lambda = 0.4$.

4. Results and discussions

It is fairly straightforward to compute the energy eigenvalues for the sSCP and the ECSC potential from our analytic expressions (2.8) to (2.11) using the appropriate values of δ and the scaling factor *a* given in (3.7) and (3.8). In tables 1-4, we present the calculated energy eigenvalues as a function of the screening parameter λ for the 1s-4s states. Our calculated values of the energy levels are compared with the accurate

		RS perturbation				
Screening parameter λ	λ/λ_{c}	Hulthén (Lam-Varshni 1971)	Scaled Hulthén	Hypervirial Padé (Lai 1981)	Variational (Lam-Varshni 1971)	Numerical (Rogers <i>et al</i> 1970)
0.10	0.08	-0.407 04	-0.407 05	-0.407 06	-0.407 06	-0.407 05
0.20	0.17	-0.326 58	-0.326 76	-0.326 81	-0.326 81	-0.326 80
0.25	0.21	-0.290 43	-0.290 83	-0.290 92	-0.290 92	-0.290 90
0.50	0.42	-0.143 58	-0.147 75	-0.148 12	-0.148 08	-0.148 10
0.80	0.67	-0.027 08	-0.044 42	-0.044 70	-0.044 59	
0.90	0.76	-0.000 09	-0.024 15	-0.024 31	-0.024 18	_
1.00	0.84	+0.021 65	-0.010 14	-0.010 27	-0.010 16	-0.010 29

Table 1. Energy eigenvalues in atomic units as a function of the screening parameter for the 1s state of the SSCP.

Table 2. Energy eigenvalues in atomic units as a function of the screening parameter for the 2s, 3s and 4s states of the SSCP.

		λ/λ_{c}	RS perturbation				
Screening parameter, λ	State		Hulthén (Lam- Varshni 1971)	Scaled Hulthén	– Hyperviral Padé (Lai 1981)	Variationa (Lam- Varshni 1971)	l Numerical (Rogers et al 1970)
0.025	3s	0.18	-0.034 30	-0.034 31	-0.034 33	-0.034 33	-0.034 33
0.025	4s	0.32	-0.012 40	-0.012 48	-0.012 50	-0.012 50	-0.012 51
0.05	2s	0.16	-0.081 73	-0.081 76	-0.081 77	-0.081 77	-0.081 77
0.05	3s	0.36	-0.019 07	-0.019 32	-0.019 35	-0.019 35	-0.019 35
0.05	4s	0.63	-0.002 23	-0.003 08	-0.003 09	-0.003 09	-0.003 09
0.06	4s	0.76	+0.000 15	-0.001 24	-0.001 24	-0.001 24	_
0.08	3s	0.57	-0.006 63	-0.007 74	-0.00778	-0.007 77	
0.10	2s	0.32	-0.049 48	-0.049 87	-0.049 93	-0.049 93	-0.049 93
0.10	3s	0.72	-0.001 09	-0.003 20	-0.003 21	-0.003 20	-0.003 21
0.11	3s	0.79	+0.000 97	-0.001 71		-0.001 72	
0.20	2s	0.64	-0.008 52	-0.012 05	-0.012 11	-0.012 08	-0.012 11
0.25	2s	0.81	+0.003 06	-0.003 32	-0.003 39	-0.003 36	-0.003 39

values obtained from the elaborate hypervirial Padé approximant scheme of Lai (1981, 1982) and variational calculation of Lam and Varshni (1971, 1972). We show here the [6, 7] and the [10, 11] Padé approximant results for the ssCP and the ECSC potential respectively. The perturbative results based on the conventional Hulthén potential as the unperturbed Hamiltonian are also shown. For the ssCP, the values obtained numerically by Rogers *et al* (1970) are given for comparison.

As can be seen from tables 1-4, the scaled Hulthén perturbation calculation gives consistently more accurate energy eigenvalues than that of the Hulthén perturbation of Lam and Varshni for large values of λ . In some cases, when the Hulthén perturbation even gives the wrong sign for the bound-state energies, our scaled Hulthén perturbation predicts fairly correct results.

		RS per	turbation			
Screening parameter, λ	λ / λ_c	Hulthén (Lam-Varshni 1972)	Scaled Hulthén	Hypervirial Padé (Lai 1982)	Variational (Lam-Varshni 1972)	
0.06	0.08	-0.440 201	-0.440 198	-0.440 201	-0.440 201	
0.08	0.11	-0.420 464	-0.420457	-0.420 464	-0.420 464	
0.10	0.14	-0.400 884	-0.400 869	-0.400 885	$-0.400\ 885$	
0.20	0.28	-0.306 298	-0.306 200	-0.306 335	-0.306 334	
0.30	0.42	-0.219 028	-0.219 044	-0.219 416	-0.219 411	
0.40	0.56	-0.140 595	-0.141 857	-0.142 439	-0.142 418	
0.50	0.69	-0.071 714	-0.077 114	-0.077 679	-0.077 606	
0.60	0.83	-0.012 585	-0.027708	-0.028 232	-0.028 031	

Table 3. Energy eigenvalues in atomic units as a function of the screening parameter for the 1s state of the ECSC potential.

Table 4. Energy eigenvalues in atomic units as a function of the screening parameter for the 2s, 3s and 4s states of the ECSC potential.

			RS pert	urbation		Variational (Lam-Varshni 1972)
Screening parameter, λ	State	λ/λ_{c}	Hulthén (Lam-Varshni 1972)	Scaled Hulthén	Hypervirial Padé (Lai 1982)	
0.02	2s	0.12	-0.105 104	-0.105 107	-0.105 104	-0.105 104
0.02	35	0.28	-0.036 024	-0.036 025	$-0.036\ 025$	-0.036 025
0.02	4s	0.49	-0.012 557	-0.012 557	-0.012 572	-0.012 572
0.03	4s	0.74		-0.005 224	-0.005 270	
0.04	2s	0.24	-0.085 768	-0.085 756	-0.085 769	-0.085 769
0.04	35	0.55	-0.018 768	-0.018 767	-0.018 823	-0.018 822
0.04	4s	0.99	+0.000670	-0.000 115	-0.000 125	-0.000 118
0.05	3s	0.69	-0.011 366	-0.011 498	-0.011 576	
0.06	2s	0.36	-0.067 408	-0.067 374	-0.067 421	-0.067 421
0.06	3s	0.83	-0.004 903	-0.005 392	-0.005 462	-0.005 454
0.07	3s	0.97	+0.000 563	-0.000 718	-0.000 750	
0.08	2s	0.48	-0.050 310	-0.050 289	-0.050 387	-0.050 384
0.10	2s	0.60	-0.034668	-0.034 794	-0.034 941	-0.034 935
0.15	2s	0.90	-0.002 566	-0.005 153	-0.005 260	_

We wish to mention at this point that it is not the value of λ only but also the ratio λ/λ_c which is important in fixing the scale of the screening for a given quantum state because the value of λ_c changes appreciably from one state to the other. The critical screening parameters for different states have been accurately determined numerically by Rogers *et al* (1970) for the ssCP and by Singh and Varshni (1983) for the ECSC potential. Using those numbers, we give the values of λ/λ_c corresponding to each value of λ in the tables. Our predicted energy eigenvalues are found to agree within 2% with the numerical and other sophisticated analytic results even when λ is as large as $0.8\lambda_c$. For the ECSC case, our result for the 4s state is also close to the variational result even when $\lambda/\lambda_c \approx 0.99$. Judged in this light the present approach therefore has

the merit of pushing the accuracy to an appreciably large value of λ/λ_c , yet remaining remarkably simple for calculated purpose.

Before we conclude, a few comments summarising the purpose and achievements of the present analysis of the scaled Hulthén perturbation would perhaps be in order. Firstly, we have derived compact analytic expressions for the energy levels which may be used for a class of screened Coulomb potentials in a unified fashion. In fact, we can predict the energy levels of the generalised exponential cosine-screened Coulomb potential (Singh and Varshni 1983) by choosing δ in (2.1) to be non-zero and different from λ . Secondly, our study has been aimed at focusing attention on some interesting aspects of the RS perturbation theory. About twelve years ago Lam and Varshni made an interesting proposition for improving the Coulomb RS perturbation calculation using the standard Hulthén potential as the unperturbed Hamiltonian. Ten years later, we have now been able to modify that idea and show that a much more accurate energy spectrum can be obtained from the RS theory on the basis of an optimally scaled zero-order Hamiltonian. In the case of the screened Coulomb potentials, it is the scaled Hulthén potential with stronger coupling and screening strengths which becomes the dominant term in the perturbation framework. The aim of this paper is not to suggest a better theoretical model than the existing ones but to demonstrate that the right choice of the unperturbed Hamiltonian in the standard RS perturbation theory predicts results in a much simpler way than by using more sophisticated and rigorous calculations.

Acknowledgment

This work has been supported in part by a research grant from the Natural Sciences and Engineering Research Council of Canada to one of the authors (YPV).

References

Bonch-Bruevich V L and Glasko V B 1959 Sov. Phys.-Dokl. 4 147 Davydov A S 1976 Quantum Mechanics (Oxford: Pergamon) Dutt R, Ray A and Ray P P 1981 Phys. Lett. 83A 65 Ecker G and Weizel W 1956 Ann. Phys., Lpz. 17 126 Gerry C C and Laub J 1984 Phys. Rev. A 30 1229 Gradshteyn I S and Ryzhik I M 1965 Tables of Integrals, Series and Products (London: Academic) Green A E S 1949 Phys. Rev. 75 1926 Harris G M 1962 Phys. Rev. 125 1131 Hall G L 1962 Phys. Chem. Solids 23 1147 Iafrate G J and Mendelsohn L B 1969 Phys. Rev. 182 244 Imbo T, Pagnamenta A and Sukhatme U 1984 University of Illinois, Chicago Preprint No UIC-84-8 Krieger J B 1969 Phys. Rev. 178 1337 Killingbeck J and Galicia S 1980 J. Phys. A: Math. Gen. 13 3419 Lam C S and Varshni Y P 1971 Phys. Rev. A 4 1875 — 1972 Phys. Rev. A 6 1391 — 1976 Phys. Lett. 59A 363 Lai C S 1981 Phys. Rev. A 23 455 - 1982 Phys. Rev. A 26 2245 Margenau H and Lewis M 1959 Rev. Mod. Phys. 31 569 McEnnan J, Kissel L and Pratt R H 1976 Phys. Rev. A 13 532 Mehta C H and Patil S H 1978 Phys. Rev. A 17 34

Moreno G and Zepeda A 1984 J. Phys. B: At. Mol. Phys. 17 21 Patil S H 1984 J. Phys. A: Math. Gen. 17 575 Ray P P and Ray A 1980 Phys. Lett. 78A 443 Rogers F J, Graboske H C Jr and Harwood D J 1970 Phys. Rev. A 1 1577 Roussel K M and O'Donnell R F 1974 Phys. Rev. A 9 52 Singh D and Varshni Y P 1983 Phys. Rev. A 28 2606 Yukawa H 1935 Proc. Phys. Math. Soc. Japan 17 48