PHYSICAL REVIEW A VOLUME 31, NUMBER 1 JANUARY 1985

Bound eigenstates for the superposition of the Coulomb and the Yukawa potentials

Janusz Adamowski
Zakład Fizyki Ciała Stałego, Akademia Górniczo-Hutnicza, PL-30-059 Kraków, Poland

(Received 30 January 1984)

The eigenvalue problem for two particles interacting through the potential being the superposition of the attractive Coulomb potential $(-A/r)$ and the Yukawa potential $B\exp(-Cr)/r$ of arbitrary strength B and screening parameter C is solved by variational means. The energy levels E_{nl} for the states 1s through 7i are calculated as functions of B and C. It is shown that for a given principal quantum number n the energy eigenvalues increase (decrease) with increasing azimuthal quantum number l if the Yukawa potential is attractive (repulsive), i.e., for $l>l'$: $E_{nl}\geq E_{nl'}$ if $B<0$, and $E_{nl}\leq E_{nl'}$ if $B>0$. It leads to the crossing of the energy levels with $n\geq 2$. For $B>0$ the levels with larger n and l become lower than those with smaller n and l, e.g., $E_{3d}<E_{2s}$, $E_{4f}<E_{2s}$, and $E_{4f}<E_{3p}$. For $B<0$ and certain intervals of C the levels with larger n but smaller l lie below those with smaller n and larger l, e.g., $E_{4s}<E_{3d}$, $E_{5s}<E_{4f}$, and $E_{5p}<E_{4f}$. The values of B and C for which the lowest-energy levels cross over are estimated. Moreover, the splitting of the 2s and 2p levels (the Lamb shift) is discussed.

I. INTRODUCTION

The eigenvalue problem for the Yukawa (Debye-Hückel) potential was considered by many authors; for example, see Refs. 1 and 2. This potential (called as well the exponentially screened Coulomb potential) describes the interaction between charge carriers in an ionized gas or in a metal. The eigenvalues of the Schrödinger equation for the Yukawa potential as well as for the exponential cosine Coulomb potential[3,4] are now well known (at least for the lowest states). The superposition of the Coulomb and the Yukawa potentials (SCYP) is an another example of the two-particle potential having applications in the solid-state physics. It was shown[5–7] that the main properties of the effective two-particle interaction for the charged particles in polar crystals are described by the SCYP. To the best of my knowledge no systematic study of the bound eigenstates for this potential was undertaken. The purpose of the present paper is therefore to calculate the lowest-lying energy levels for the SCYP and to study their properties.

II. SOLUTION OF THE SCHRÖDINGER EQUATION

We consider a two-particle system interacting through the potential (SCYP)

$$V(r)=-\frac{A}{r}+\frac{B}{r}e^{-Cr}\;, \tag{1}$$

where r is the distance between the particles, A and B are the strengths of the Coulomb and the Yukawa potentials, respectively, and C is the screening parameter ($C=1/D$, where D is the screening length). We assume that A and C are positive. The radial Schrödinger equation has the form

$$\left[-\frac{d^2}{dr^2}-\frac{2}{r}\frac{d}{dr}+\frac{l(l+1)}{r^2}-\frac{2}{r}+\frac{B}{r}e^{-Cr}\right]R(r)=ER(r)\;, \tag{2}$$

where the length has been expressed in units of $a_0=\hbar^2/\mu A$, the energy in units of $E_0=\mu A^2/2\hbar^2$, and μ is the reduced mass of the two particles. In Eq. (2) all quantities are dimensionless, in particular, the parameters of the potential have been changed with respect to those in Eq. (1) as follows: $B'=2B/A$ and $C'=Ca_0$, and next the primes have been omitted. The units E_0 and a_0 will be used throughout this paper.

The Schrödinger equation (2) is not solvable analytically. Nevertheless, some properties of its eigenvalues can be guessed without solving it. The bound eigenstates exist for all values of the parameters B and C. For $B\leq 2$ the bound eigenstates appear since the potential is attractive for all r and has the long-range Coulomb tail. For $B=2$ the potential takes on the finite value at $r=0$: $V(0)=-2C$, and next increases to zero when $r\to\infty$. For $B>2$ the potential is repulsive for small r, but it goes through zero for $r_0=-(1/C)\ln(2/B)$ and has a minimum for $r>r_0$. At large distances the Coulomb part also dominates. Such a potential provides the bound states for all B and C only if $C\geq 0$. The degeneracy of the energy levels with the same principal quantum number n and with different azimuthal quantum numbers l, peculiar to the purely Coulombic potential, vanishes. Therefore, the energy eigenvalues depend on both the quantum numbers n and l. They become hydrogenlike in the limits: (i) if $C\to\infty$ and/or $B\to 0$, then $E_{nl}\to E_n^{\mathrm{H}}$, where

$$E_n^{\mathrm{H}}=-\frac{1}{n^2}\;; \tag{3}$$

and (ii) if $C\to 0$ and $B<2$, then $E_{nl}\to E_n^0$, where

$$E_n^0=-BC-\frac{(B-2)^2}{4n^2}\;. \tag{4}$$

Expressions (3) and (4) provide the upper or lower bounds to the energy eigenvalues E_{nl} of Eq. (2) if $B<0$ or $B>0$, respectively. The bounds E_n^0 are valid for $B<2$.

To solve the Schrödinger equation (2) the following wave function has been used:

$$R(r)=\sum_{j=1}^{N}\frac{c_j}{\sqrt{N_j}}e^{-\gamma_j r}\,, \tag{5}$$

where c_j and γ_j are the variational parameters, and the normalization constants $N_j=1/4\gamma_j^3$. I used the $N=10$ element basis with one nonlinear variational parameter γ, where $\gamma_j=j\gamma$. The parameters c_j are obtained from the diagonalization procedure. They take on such values that for each state the wave function (5) is normalized and orthogonal to the corresponding wave functions for the states with the same l and different n. This enables us to use the variational method for the discrete spectrum.[8] Trial function (5) was examined for the eigenvalue problems for the Coulomb and the Yukawa potentials. The eigenvalues calculated with the help of (5) reproduce the analytical results for the Coulomb potential up to the level $n=7$ and the numerical results[1,2] for the Yukawa potential up to the level $7i$. Therefore, one can expect that the trial wave function (5) provides the lowest eigenvalues of Eq. (2) with a sufficient precision.

III. RESULTS

Tables I, II, and III show the calculated energy eigenvalues of the lowest-lying states (from $1s$ up to $4f$) for $B=\pm1$, ±2, and ±4 as functions of the screening parameter C. Tables IV and V contain the results for the strongly repulsive ($B=10$) and strongly attractive ($B=-10$) Yukawa potentials. The dependence of the energy levels on B is shown on Fig. 1 for the states $2s$ and $2p$ and in Tables VI–VIII for the states $1s$–$3d$. The results for the higher excited states (from $5s$ up to $7i$) are presented in Table IX. The energy eigenvalues $1s$–$6h$ for the attractive Yukawa potential with $C=1$ as functions of B are shown in Table X.

The present calculations show that the spectra of the SCYP possess the following properties.

(i) For a given n the energy eigenvalues E_{nl} increase with increasing l if the Yukawa potential is attractive, and E_{nl} decrease with increasing l if the Yukawa potential is repulsive; i.e., for $l>l'$, $E_{nl}-E_{nl'}\geq 0$ or $E_{nl}-E_{nl'}\leq 0$ if $B<0$ or $B>0$, respectively.

(ii) For the repulsive Yukawa potential there are some values of the strength B and the screening parameter C for which the energy eigenvalues for larger n and l become lower than those for smaller n and l, i.e., $E_{nl}\leq E_{n'l'}$ if $n>n'\geq 2$ and $l>l'$.

(iii) For the attractive Yukawa potential there exist some values of B and C for which the energy levels with larger n and smaller l become lower than the levels with smaller n and larger l, i.e., $E_{nl}\leq E_{n'l'}$ if $n>n'\geq 3$ and $l<l'$.

Figure 2 is an illustration of property (i). It shows the positions of the energy levels with respect to the corresponding hydrogenlike levels E_n^{H} [Eq. (3)] as functions of the azimuthal quantum number l for $n=5$, 6, and 7, $B=\pm10$, and $C=0.1$. For each n the absolute values of the differences $|E_{nl}-E_n^{\mathrm{H}}|$ are decreasing functions of l. The s levels are mostly split off from E_n^{H} (downwards for $B<0$ and upwards for $B>0$). The energy eigenvalues E_{nl} approach E_n^{H} if n and l increase. This property can be understood if we consider the unperturbed wave function $R_{nl}^{\mathrm{H}}(r)$, i.e., the eigenfunction of Eq. (2) for $B=0$, which varies like r^l for small r. The shift of the energy levels with respect to E_n^{H} is due to an influence of the finite-range Yukawa potential. Therefore, this shift is larger as the larger values are taken on by $R_{nl}^{\mathrm{H}}(r)$ at small distances. The wave function [Eq. (5)] obtained in the present calcu-

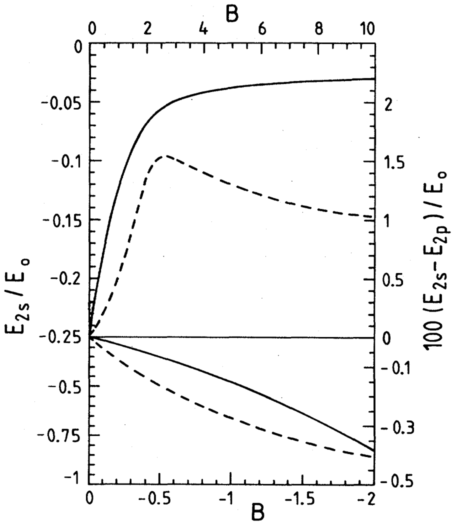

FIG. 1. Energy of the $2s$ state (solid curves) and $2s$-$2p$ splitting (dashed curves) as functions of the strength B of the Yukawa potential with the screening parameter $C=0.1$. Straight line shows the results for the $n=2$ level of the purely Coulombic potential ($-2/r$). The unit of energy is $E_0=\mu A^2/2\hbar^2$.

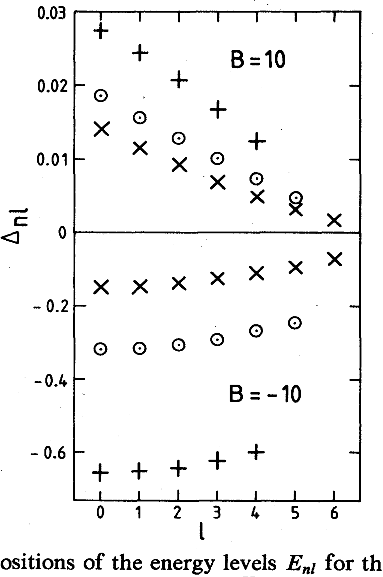

FIG. 2. Positions of the energy levels E_{nl} for the SCYP with respect to the hydrogenlike levels $E_n^{\mathrm{H}}=-1/n^2$, $\Delta_{nl}=E_{nl}-E_n^{\mathrm{H}}$, as functions of the azimuthal quantum number l for $C=0.1$ and $B=\pm10$. Energy is expressed in units of $E_0=\mu A^2/2\hbar^2$, the results for $n=5$ are labeled by $+$, for $n=6$ by $\odot$, and for $n=7$ by $\times$.

TABLE I. Energy eigenvalues of states 1*s*—4*f* for the superposition of the Coulomb potential and the Yukawa potential as functions of the screening parameter C for $B=\pm 1$. Energy is expressed in units of $E_0=\mu A^2/2\hbar^2$, length in units of $a_0=\hbar^2/\mu A$, and μ is the reduced mass of the interacting particles.

C State	0.001	0.005	0.01	0.05	0.1	0.2	0.5	1	2	10
					$B=+1$					
1*s*	−0.251 00	−0.254 96	−0.259 85	−0.296 50	−0.336 94	−0.404 24	−0.542 43	−0.674 82	−0.805 66	−0.974 24
2*s*	−0.063 49	−0.067 35	−0.071 93	−0.100 71	−0.124 36	−0.152 54	−0.187 81	−0.208 88	−0.225 81	−0.245 78
2*p*	−0.063 50	−0.067 38	−0.072 02	−0.102 42	−0.129 31	−0.164 29	−0.212 03	−0.236 65	−0.247 11	−0.249 98
3*s*	−0.028 76	−0.032 46	−0.036 56	−0.057 17	−0.069 52	−0.080 83	−0.092 14	−0.098 69	−0.103 87	−0.110 15
3*p*	−0.028 77	−0.032 48	−0.036 64	−0.053 68	−0.072 42	−0.086 33	−0.100 52	−0.107 00	−0.110 17	−0.111 11
3*d*	−0.028 77	−0.032 52	−0.036 81	−0.060 52	−0.077 05	−0.093 73	−0.107 70	−0.110 67	−0.111 08	−0.111 11
4*s*	−0.016 60	−0.020 08	−0.023 64	−0.037 86	−0.044 31	−0.049 40	−0.054 28	−0.057 26	−0.059 36	−0.062 09
4*p*	−0.016 60	−0.020 10	−0.023 71	−0.038 69	−0.046 04	−0.052 13	−0.058 01	−0.060 80	−0.062 09	−0.062 50
4*d*	−0.016 60	−0.020 14	−0.023 86	−0.040 14	−0.048 69	−0.055 66	−0.060 98	−0.062 27	−0.062 48	−0.062 50
4*f*	−0.016 61	−0.020 21	−0.024 07	−0.042 00	−0.051 71	−0.059 00	−0.062 27	−0.062 49	−0.062 50	−0.062 50
					$B=-1$					
1*s*	−2.249 00	−2.245 01	−2.240 05	−2.201 22	−2.154 79	−2.068 40	−1.853 02	−1.601 49	−1.328 71	−1.030 13
2*s*	−0.561 50	−0.557 55	−0.552 70	−0.517 14	−0.479 84	−0.423 73	−0.340 92	−0.302 13	−0.281 22	−0.253 67
2*p*	−0.561 50	−0.557 54	−0.552 66	−0.516 41	−0.477 27	−0.415 69	−0.316 64	−0.268 79	−0.253 32	−0.250 02
3*s*	−0.249 00	−0.245 11	−0.240 44	−0.209 63	−0.183 60	−0.155 79	−0.133 47	−0.125 31	−0.119 91	−0.112 19
3*p*	−0.249 00	−0.245 10	−0.240 40	−0.209 00	−0.181 72	−0.151 44	−0.125 96	−0.116 35	−0.112 19	−0.111 12
3*d*	−0.249 00	−0.245 09	−0.240 34	−0.207 75	−0.117 94	−0.142 88	−0.115 61	−0.111 58	−0.111 14	−0.111 11
4*s*	−0.139 63	−0.135 82	−0.131 38	−0.106 02	−0.090 15	−0.078 69	−0.071 39	−0.068 30	−0.066 13	−0.062 95
4*p*	−0.139 63	−0.135 81	−0.131 35	−0.105 52	−0.088 93	−0.076 61	−0.068 34	−0.064 68	−0.062 97	−0.062 50
4*d*	−0.139 63	−0.135 80	−0.131 29	−0.104 52	−0.086 50	−0.072 72	−0.064 45	−0.062 75	−0.062 52	−0.062 50
4*f*	−0.139 63	−0.135 77	−0.131 20	−0.103 01	−0.082 88	−0.067 81	−0.062 76	−0.062 51	−0.062 50	−0.062 50

TABLE II. Energy eigenvalues for $B=\pm 2$. Symbols have the same meaning as in Table I.

C State	0.001	0.005	0.01	0.05	0.1	0.2	0.5	1	2	10
					$B=+2$					
1*s*	−0.001 78	−0.008 14	−0.015 40	−0.063 25	−0.111 30	−0.188 47	−0.348 91	−0.512 46	−0.688 56	−0.951 97
2*s*	−0.001 62	−0.006 93	−0.012 51	−0.043 40	−0.068 26	−0.100 13	−0.146 97	−0.180 06	−0.208 14	−0.243 93
2*p*	−0.001 68	−0.007 39	−0.013 60	−0.050 19	−0.081 88	−0.124 86	−0.189 15	−0.226 68	−0.244 58	−0.249 97
3*s*	−0.001 50	−0.006 04	−0.010 48	−0.031 37	−0.044 93	−0.059 60	−0.077 69	−0.089 16	−0.098 30	−0.109 30
3*p*	−0.001 55	−0.006 41	−0.011 31	−0.035 79	−0.052 81	−0.071 59	−0.093 12	−0.103 98	−0.109 34	−0.111 10
3*d*	−0.001 60	−0.006 78	−0.012 15	−0.040 39	−0.061 00	−0.083 60	−0.105 02	−0.110 27	−0.111 06	−0.111 11
4*s*	−0.001 40	−0.005 32	−0.008 91	−0.023 41	−0.031 32	−0.038 94	−0.047 67	−0.052 87	−0.056 93	−0.061 73
4*p*	−0.001 44	−0.005 63	−0.009 57	−0.026 42	−0.036 04	−0.045 21	−0.054 74	−0.059 44	−0.061 73	−0.062 49
4*d*	−0.001 50	−0.005 94	−0.010 24	−0.029 51	−0.040 85	−0.051 11	−0.059 74	−0.062 06	−0.062 47	−0.062 50
4*f*	−0.001 54	−0.006 26	−0.010 92	−0.032 70	−0.045 69	−0.056 45	−0.062 05	−0.062 48	−0.062 50	−0.062 50
					$B=-2$					
1*s*	−3.998 00	−3.990 02	−3.980 07	−3.901 84	−3.807 26	−3.628 17	−3.162 02	−2.574 23	−1.869 04	−1.065 78
2*s*	−0.998 00	−0.990 07	−0.980 30	−0.907 09	−0.826 95	−0.698 09	−0.480 18	−0.366 65	−0.318 09	−0.257 89
2*p*	−0.998 00	−0.990 06	−0.980 25	−0.905 96	−0.822 83	−0.684 45	−0.432 74	−0.296 74	−0.257 21	−0.250 03
3*s*	−0.442 45	−0.434 61	−0.425 10	−0.359 45	−0.298 61	−0.224 89	−0.160 31	−0.140 75	−0.129 67	−0.113 41
3*p*	−0.442 45	−0.434 60	−0.425 05	−0.358 45	−0.295 38	−0.216 62	−0.145 72	−0.123 38	−0.113 44	−0.111 12
3*d*	−0.442 45	−0.434 57	−0.424 96	−0.356 44	−0.288 85	−0.199 75	−0.121 89	−0.112 11	−0.111 17	−0.111 11
4*s*	−0.248 01	−0.240 29	−0.231 15	−0.174 64	−0.133 51	−0.100 03	−0.081 11	−0.074 30	−0.070 03	−0.063 45
4*p*	−0.248 01	−0.240 28	−0.2 31	−0.173 79	−0.131 23	−0.095 94	−0.075 54	−0.067 50	−0.063 50	−0.062 51
4*d*	−0.248 01	−0.240 26	−0.231 01	−0.172 09	−0.126 63	−0.087 90	−0.067 02	−0.063 02	−0.062 53	−0.062 50
4*f*	−0.248 01	−0.240 22	−0.230 87	−0.169 52	−0.119 60	−0.076 53	−0.063 04	−0.062 52	−0.062 50	−0.062 50

TABLE III. Energy eigenvalues for $B=\pm4$. Symbols have the same meaning as in Table I.

C State	0.001	0.005	0.01	0.05	0.1	0.2	0.5	1	2	10
					$B=+4$					
1s	−0.000 727	−0.003 59	−0.007 00	−0.032 35	−0.060 88	−0.111 60	−0.233 59	−0.379 84	−0.564 07	−0.915 40
2s	−0.000 676	−0.003 23	−0.006 15	−0.024 65	−0.041 73	−0.066 84	−0.111 24	−0.149 35	−0.185 98	−0.239 14
2p	−0.000 726	−0.003 55	−0.006 94	−0.030 90	−0.055 70	−0.094 51	−0.163 80	−0.212 70	−0.240 29	−0.249 93
3s	−0.000 603	−0.002 83	−0.005 32	−0.018 80	−0.029 70	−0.043 09	−0.063 15	−0.078 05	−0.090 94	−0.107 83
3p	−0.000 676	−0.003 21	−0.006 10	−0.023 57	−0.038 44	−0.057 49	−0.083 92	−0.099 40	−0.107 92	−0.111 09
3d	−0.000 725	−0.003 51	−0.006 81	−0.028 40	−0.047 82	−0.072 60	−0.100 98	−0.109 54	−0.111 01	−0.111 11
4s	−0.000 508	−0.002 39	−0.004 44	−0.014 88	−0.021 89	−0.029 77	−0.040 46	−0.047 75	−0.053 64	−0.061 09
4p	−0.000 602	−0.002 81	−0.005 26	−0.018 25	−0.027 49	−0.037 87	−0.050 55	−0.057 37	−0.061 11	−0.062 49
4d	−0.000 674	−0.003 18	−0.005 98	−0.021 73	−0.033 32	−0.045 68	−0.057 86	−0.061 68	−0.062 44	−0.062 50
4f	−0.000 723	−0.003 46	−0.006 63	−0.025 36	−0.039 35	−0.053 01	−0.061 66	−0.062 46	−0.062 50	−0.062 50
					$B=-4$					
1s	−8.996 00	−8.980 03	−8.960 10	−8.801 47	−8.609 79	−8.238 34	−7.226 33	−5.832 64	−3.887 87	−1.160 58
2s	−2.246 00	−2.230 10	−2.210 40	−2.059 63	−1.887 20	−1.589 49	−0.987 45	−0.568 51	−0.402 01	−0.268 48
2p	−2.246 00	−2.230 08	−2.210 33	−2.058 04	−1.881 35	−1.568 87	−0.900 50	−0.411 74	−0.267 79	−0.250 07
3s	−0.996 01	−0.980 22	−0.960 89	−0.820 79	−0.677 49	−0.473 53	−0.237 67	−0.176 78	−0.149 80	−0.116 41
3p	−0.996 01	−0.980 21	−0.960 82	−0.819 35	−0.672 52	−0.458 83	−0.206 27	−0.144 65	−0.116 69	−0.111 14
3d	−0.996 01	−0.980 17	−0.960 69	−0.816 46	−0.662 48	−0.428 61	−0.146 50	−0.113 34	−0.111 22	−0.111 11
4s	−0.558 52	−0.542 89	−0.524 05	−0.397 49	−0.287 49	−0.172 11	−0.104 06	−0.087 17	−0.077 69	−0.064 62
4p	−0.558 52	−0.542 88	−0.523 99	−0.396 21	−0.283 56	−0.163 53	−0.093 69	−0.075 50	−0.064 88	−0.062 51
4d	−0.558 51	−0.542 85	−0.523 86	−0.393 64	−0.275 62	−0.146 08	−0.075 39	−0.063 67	−0.062 56	−0.062 50
4f	−0.558 51	−0.542 80	−0.523 67	−0.389 75	−0.263 43	−0.118 98	−0.063 70	−0.062 54	−0.062 50	−0.062 50

TABLE IV. Energy eigenvalues for $B=10$. Symbols have the same meaning as in Table I.

C State	0.001	0.005	0.01	0.05	0.1	0.2	0.5	1	2	10
1s	−0.000 481	−0.002 38	−0.004 70	−0.021 98	−0.041 66	−0.077 17	−0.165 61	−0.278 79	−0.437 54	−0.843 95
2s	−0.000 428	−0.002 09	−0.004 06	−0.017 14	−0.029 63	−0.048 64	−0.085 27	−0.120 66	−0.159 19	−0.229 28
2p	−0.000 481	−0.002 37	−0.004 68	−0.021 50	−0.039 87	−0.070 77	−0.134 73	−0.190 81	−0.231 26	−0.249 84
3s	−0.000 339	−0.001 66	−0.003 35	−0.013 40	−0.021 81	−0.032 91	−0.051 28	−0.066 59	−0.081 39	−0.104 77
3p	−0.000 427	−0.002 08	−0.004 04	−0.016 77	−0.028 43	−0.044 98	−0.072 20	−0.091 82	−0.104 92	−0.111 05
3d	−0.000 481	−0.002 36	−0.004 64	−0.020 58	−0.036 60	−0.060 03	−0.093 88	−0.107 82	−0.110 86	−0.111 11
4s	−0.000 274	−0.001 34	−0.002 60	−0.010 07	−0.016 14	−0.023 64	−0.034 13	−0.042 10	−0.049 26	−0.059 74
4p	−0.000 339	−0.00165	−0.003 34	−0.013 11	−0.020 70	−0.030 74	−0.044 83	−0.053 92	−0.059 78	−0.062 47
4d	−0.000 427	−0.002 07	−0.003 97	−0.016 07	−0.026 23	−0.038 87	−0.054 46	−0.060 80	−0.062 36	−0.062 50
4f	−0.000 480	−0.002 35	−0.004 58	−0.019 30	−0.032 34	−0.047 74	−0.063 70	−0.062 41	−0.062 50	−0.062 50

TABLE V. Energy eigenvalues for $B=-10$. Symbols have the same meaning as in Table I.

C State	0.01	0.05	0.1	0.2	0.5	0.85	1.25	1.55	2	10
1s	−35.9001	−35.5031	−35.0124	−34.0489	−31.2967	−28.3300	−25.2339	−23.1021	−20.1860	−1.9577
2s	−8.9005	−8.5122	−8.0482	−7.1862	−5.0617	−3.2972	−2.0004	−1.4049	−0.9167	−0.3336
2p	−8.9004	−8.5102	−8.0404	−7.1569	−4.9105	−2.9522	−1.4597	−0.7972	−0.3821	−0.2502
3s	−3.9011	−3.5270	−3.1040	−2.3887	−1.0452	−0.4542	−0.2968	−0.2595	−0.2259	−0.1335
3p	−3.9010	−3.5251	−3.0968	−2.3638	−0.9507	−0.3367	−0.2111	−0.1833	−0.1454	−0.1112
3d	−3.9009	−3.5212	−3.0824	−2.3136	−0.7516	−0.1413	−0.1140	−0.1121	−0.1114	−0.1111
4s	−2.1520	−1.7966	−1.4254	−0.8800	−0.2431	−0.1503	−0.1227	−0.1130	−0.1032	−0.0712
4p	−2.1519	−1.7948	−1.4190	−0.8606	−0.2063	−0.1233	−0.0979	−0.0890	−0.0762	−0.0625
4d	−2.1517	−1.7912	−1.4061	−0.8210	−0.1384	−0.0767	−0.0641	−0.0631	−0.0627	−0.0625
4f	−2.1515	−1.7856	−1.3866	−0.7598	−0.0681	−0.0628	−0.0625	−0.0625	−0.0625	−0.0625

TABLE VI. Energy eigenvalues of states $1s-3d$ as functions of the strength B of the Yukawa potential for $C=0.25$. Symbols have the same meaning as in Table I.

State B	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$
100	−0.055 97	−0.036 15	−0.053 27	−0.025 33	−0.034 60	−0.048 19
20	−0.077 27	−0.047 70	−0.071 38	−0.032 05	−0.044 56	−0.061 09
10	−0.093 52	−0.056 27	−0.080 03	−0.036 91	−0.051 17	−0.068 67
5	−0.120 92	−0.070 06	−0.102 36	−0.044 45	−0.060 48	−0.077 62
2	−0.221 05	−0.111 41	−0.140 49	−0.064 27	−0.077 39	−0.090 22
1	−0.432 75	−0.161 72	−0.176 43	−0.083 96	−0.090 35	−0.098 28
0.5	−0.662 22	−0.199 81	−0.206 70	−0.096 59	−0.099 57	−0.103 89
0.2	−0.851 25	−0.228 21	−0.230 85	−0.105 04	−0.106 19	−0.107 99
−0.2	−1.167 40	−0.274 38	−0.271 90	−0.117 57	−0.116 48	−0.114 59
−0.5	−1.454 07	−0.316 39	−0.310 43	−0.128 11	−0.125 44	−0.120 59
−1	−2.028 20	−0.402 77	−0.391 66	−0.148 49	−0.143 24	−0.133 20
−2	−3.543 38	−0.646 66	−0.627 29	−0.203 59	−0.193 32	−0.172 51
−5	−11.0640	−2.044 20	−2.010 28	−0.562 80	−0.539 39	−0.490 98
−10	−33.5761	−6.786 15	−6.741 84	−2.088 53	−2.052 53	−1.979 22
−20	−116.084	−25.5743	−25.5223	−9.136 22	−9.089 73	−8.996 11

TABLE VII. Energy eigenvalues for $C=0.75$. Symbols have the same meaning as in Tables I and VI.

State B	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$
100	−0.139 28	−0.072 28	−0.120 48	−0.044 82	−0.065 02	−0.090 26
20	−0.189 09	−0.092 03	−0.150 77	−0.054 12	−0.077 46	−0.100 17
10	−0.226 23	−0.105 35	−0.168 13	−0.060 19	−0.084 19	−0.103 79
5	−0.285 78	−0.124 98	−0.187 79	−0.068 59	−0.091 43	−0.106 61
2	−0.441 23	−0.166 82	−0.213 33	−0.084 67	−0.100 14	−0.109 00
1	−0.618 37	−0.200 71	−0.228 23	−0.096 16	−0.104 82	−0.109 99
0.5	−0.775 11	−0.223 50	−0.238 01	−0.103 30	−0.107 72	−0.110 53
0.2	−0.900 79	−0.238 96	−0.244 89	−0.107 92	−0.109 69	−0.110 87
−0.2	−1.111 27	−0.261 63	−0.255 58	−0.114 38	−0.112 62	−0.111 36
−0.5	−1.308 72	−0.280 26	−0.264 95	−0.119 43	−0.115 07	−0.111 74
−1	−1.713 43	−0.314 96	−0.283 87	−0.128 21	−0.119 70	−0.112 42
−2	−2.842 40	−0.403 52	−0.339 40	−0.147 44	−0.131 23	−0.113 96
−5	−9.032 47	−0.974 75	−0.806 43	−0.224 51	−0.183 90	−0.121 23
−10	−29.1520	−3.733 55	−3.445 36	−0.553 40	−0.432 62	−0.198 11
−20	−106.735	−17.9288	−17.5354	−3.741 19	−3.470 08	−2.901 89

TABLE VIII. Energy eigenvalues for $C=1.5$. Symbols have the same meaning as in Tables I and VI.

State B	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$
100	−0.232 86	−0.104 67	−0.176 65	−0.059 56	−0.086 08	−0.106 94
20	−0.310 61	−0.128 02	−0.205 05	−0.069 42	−0.096 21	−0.109 69
10	−0.366 53	−0.143 43	−0.217 61	−0.075 43	−0.100 52	−0.110 31
5	−0.449 90	−0.163 50	−0.228 75	−0.083 10	−0.104 26	−0.110 68
2	−0.616 31	−0.197 22	−0.239 40	−0.094 81	−0.107 74	−0.110 93
1	−0.753 52	−0.219 25	−0.244 21	−0.101 88	−0.109 28	−0.111 02
0.5	−0.858 58	−0.233 49	−0.246 96	−0.106 24	−0.110 15	−0.111 06
0.2	−0.938 37	−0.243 13	−0.248 75	−0.109 10	−0.110 72	−0.111 09
−0.2	−1.069 24	−0.257 21	−0.251 31	−0.113 19	−0.111 52	−0.111 13
−0.5	−1.189 07	−0.268 61	−0.253 38	−0.116 41	−0.112 16	−0.111 16
−1	−1.437 88	−0.289 02	−0.257 16	−0.122 00	−0.113 33	−0.111 21
−2	−2.160 40	−0.334 24	−0.266 29	−0.133 66	−0.116 07	−0.111 31
−5	−6.676 43	−0.521 76	−0.319 41	−0.172 48	−0.130 20	−0.111 63
−10	−23.4466	−1.486 01	−0.882 80	−0.264 35	−0.187 49	−0.112 31
−20	−93.8292	−9.870 58	−8.676 43	−0.790 76	−0.443 77	−0.115 19

TABLE IX. Energy eigenvalues of states $5s-7i$ for $C=0.1$. Symbols have the same meaning as in Table I.

State \ B	+1	−1	+2	−2	+4	−4
$5s$	−0.030 49	−0.052 52	−0.022 82	−0.070 36	−0.016 56	−0.134 21
$5p$	−0.031 55	−0.051 79	−0.025 80	−0.068 92	−0.020 12	−0.131 39
$5d$	−0.033 13	−0.050 30	−0.028 74	−0.066 04	−0.024 15	−0.125 68
$5f$	−0.034 87	−0.048 25	−0.031 61	−0.061 72	−0.027 86	−0.116 92
$5g$	−0.036 59	−0.045 70	−0.034 32	−0.055 97	−0.031 52	−0.104 81
$6s$	−0.022 18	−0.034 46	−0.017 25	−0.042 93	−0.012 75	−0.070 08
$6p$	−0.022 84	−0.034 02	−0.018 93	−0.042 07	−0.015 60	−0.068 26
$6d$	−0.023 83	−0.033 16	−0.021 16	−0.040 39	−0.018 15	−0.064 62
$6f$	−0.024 90	−0.031 97	−0.022 93	−0.037 92	−0.020 56	−0.059 13
$6g$	−0.025 89	−0.030 57	−0.024 56	−0.034 80	−0.022 81	−0.051 74
$6h$	−0.026 76	−0.029 22	−0.025 98	−0.031 43	−0.024 86	−0.042 38
$7s$	−0.016 76	−0.024 41	−0.013 28	−0.028 94	−0.009 36	−0.042 11
$7p$	−0.017 24	−0.024 13	−0.014 77	−0.028 43	−0.011 93	−0.041 03
$7d$	−0.017 90	−0.023 60	−0.016 12	−0.027 59	−0.014 00	−0.038 91
$7f$	−0.018 61	−0.022 88	−0.017 32	−0.026 12	−0.015 71	−0.035 78
$7g$	−0.019 23	−0.022 06	−0.018 37	−0.024 37	−0.017 20	−0.031 76
$7h$	−0.019 75	−0.021 29	−0.019 24	−0.022 55	−0.018 48	−0.027 09
$7i$	−0.020 13	−0.020 75	−0.019 89	−0.021 18	−0.019 51	−0.022 60

lations has a similar shape to that of $R_{nl}^{\mathrm{H}}(r)$ if the Yukawa contribution is not large.

Table XI shows the critical values C_0, C_1, and C_2, for which the levels $2s-4f$ (for $B>0$) and $3d-5p$ (for $B<0$) cross over. For positive B and for $C \le C_0$ the state with the larger principal quantum number n has lower energy than that with smaller n. For higher excited states the level crossing takes place at smaller B, e.g., $E_{7i} < E_{6s}$ up to $B=1.25$. For $0<B<1.25$ no level crossing between the levels $2s-7i$ has been obtained. With increasing B the number of energy levels with different n and l, which cross over, increases. An interesting feature of the spectra for the positive strength B is that the energy eigenvalues of the states $2p$, $3d$, $4f$, etc. tend to E_{1s} with increasing B and decreasing C and in the limit they become degenerate with the state $1s$ (see Table IV). It should be noted that the states $1s, 2p, 3d, 4f, \ldots$ are the lowest eigenstates with the orbital momentum quantum numbers $l=0,1,2,3,\ldots$, respectively.

For negative B one can observe an opposite tendency. The levels E_{4s}, E_{5s}, etc. lie below the E_{3d}, E_{4f}, etc., respectively, if the values of the screening parameter be-

TABLE X. Energy eigenvalues of states $1s-6h$ for $C=1$. Symbols have the same meaning as in Table I.

State \ B	−5	−8	−10	−20	−30	−50
$1s$	−8.1637	−18.0693	−27.1336	−102.2894	−227.3520	−627.4070
$2s$	−0.7334	−1.6570	−2.7323	−14.8343	−38.9624	−124.3203
$2p$	−0.5265	−1.3061	−2.3053	−14.1939	−38.2253	−123.4919
$3s$	−0.1981	−0.2800	−0.3652	−2.2297	−8.3499	−36.1419
$3p$	−0.1588	−0.2099	−0.2605	−1.8634	−7.8233	−35.4589
$3d$	−0.1141	−0.1171	−0.1207	−1.0866	−6.7237	−34.0663
$4s$	−0.0942	−0.1178	−0.1368	−0.3142	−1.2721	−10.0259
$4p$	−0.0805	−0.0971	−0.1105	−0.2274	−1.0059	−9.5239
$4d$	−0.0641	−0.0657	−0.0677	−0.1161	−0.4802	−8.1119
$4f$	−0.0625	−0.0626	−0.0626	−0.0627	−0.0630	−6.8572
$5s$	−0.0550	−0.0649	−0.0723	−0.1230	−0.2234	−1.9100
$5p$	−0.0487	−0.0561	−0.0617	−0.0997	−0.1711	−1.6225
$5d$	−0.0409	−0.0418	−0.0429	−0.0646	−0.1032	−1.0472
$5f$	−0.0400	−0.0401	−0.0401	−0.0402	−0.0404	−0.2035
$5g$	−0.0400	−0.0400	−0.0400	−0.0400	−0.0400	−0.0400
$6s$	−0.0359	−0.0409	−0.0443	−0.0639	−0.0944	−0.2673
$6p$	−0.0324	−0.0365	−0.0392	−0.0552	−0.0786	−0.1287
$6d$	−0.0283	−0.0288	−0.0295	−0.0410	−0.0583	−0.1106
$6f$	−0.0278	−0.0278	−0.0278	−0.0279	−0.0281	−0.0601
$6g$	−0.0278	−0.0278	−0.0278	−0.0278	−0.0278	−0.0278
$6h$	−0.0278	−0.0278	−0.0278	−0.0278	−0.0278	−0.0278

TABLE XI. Estimated critical values of the screening parameter C for the crossing of the energy levels $n\,l$-$n'l'$ as functions of the strength B. For positive B the level $n'l'$ is located below the level nl if $C \le C_0$. C_0 is listed in the upper part of the table. For negative B the level $n'l'$ lies below the level nl if $C_1 \le C \le C_2$. C_1 is the first number, and C_2 the second quoted for each pair nl-$n'l'$ in the lower part of the table.

B	$2s$-$4f$	$3p$-$4f$	$3s$-$4d$	$2s$-$3d$	$3s$-$4f$
2					0.12
4	0.07	0.12	0.30	0.33	0.46
10	0.18	0.27	0.68	0.71	0.82

B	$3d$-$4s$		$4f$-$5s$		$4f$-$5p$	
-8	0.83	1.02	0.36	1.14	0.37	0.74
-10	0.82	1.58	0.40	1.56	0.41	0.97
-20	1.21	3.92	0.63	3.38	0.64	1.88
-50	2.57	8.84	1.37	6.51	1.39	4.22

long to the interval $C_1 \le C \le C_2$ and if $|B|$ is large enough. The values C_1 and C_2 for the crossing of the energy levels $3d$-$4s$, $4f$-$5s$, and $4f$-$5p$ are given in Table XI for several values of B. The crossing between the levels $3d$-$4s$ and $4f$-$5s$ has been obtained for $B \le -7.78$ and -4.58, respectively. The calculations of the lowest energy levels were performed for $-100 \le B \le 100\,000$ and $0.001 \le C \le 100$ and in these limits the properties (i)–(iii) were confirmed.

The splitting of the $2s$ and $2p$ levels, which corresponds to the Lamb shift in the hydrogen atom,[9] is shown on Fig. 1. The Lamb shift $E_{2s}-E_{2p}$ is positive if the Yukawa potential is repulsive and for $C=0.1$ takes a maximum if $B=2.65$. For B negative the Lamb shift is negative, too, and changes monotonically with B. It seems that this property, that the Lamb shift has the same sign as the potential superposed with the Coulomb one, holds true for a much broader class of potentials. One can show by the first-order perturbation theory that this is valid for the δ-like potential $\lambda\delta(r)/r^2$ and for the potentials of the form λr^{ν} if $\nu>0$ or $-2 \le \nu < -1$. These potentials superposed with the attractive Coulomb potential lead to the Lamb shift of the same sign as the sign of their strength λ (at least for small λ). It agrees with the theorems[10,11] stating that for $\lambda>0$ and $\nu>0$, $E_{2p}<E_{2s}<E_{3d}$. For $-1<\nu<0$ and small λ the Lamb shift has a sign opposite to λ.

Approximate analytical expressions for the energy eigenvalues of the SCYP can be found with the help the hydrogenic wave functions $R_{nl}^{\mathrm{H}}(r)$. They are, for the $2s$ state,

$$E_{2s}^{(1)} = -\frac{1}{4}\left[1-\frac{B(2C^2+1)}{(C+1)^4}\right], \tag{6a}$$

and for the states with $l=n-1$, i.e., the states with the lowest energy for each l,

$$E_{n,n-1}^{(1)} = -\frac{1}{n^2}\left[1-\frac{B}{(\frac{1}{2}nC+1)^{2n}}\right]. \tag{6b}$$

Formulas (6) provide the upper bounds to the energy levels of the SCYP for all values of B and C, but are useful for $C \gg 1$ or $|B| \ll 1$. If $C \to \infty$ the bounds (6) go over into $E_n^{(1)}=E_n^{\mathrm{H}}=-1/n^2$ [Eq. (3)]. On the other hand, using the wave functions for the potential $(B-2)/2r$ we obtain the following upper bounds, which are valid only for $B<2$:

$$E_{2s}^{(2)} = \frac{B-2}{16}\left[2+B-\frac{2B(2-B)^2[8C^2+(2-B)^2]}{(2C+2-B)^4}\right] \tag{7a}$$

and, for the states with $l=n-1$,

TABLE XII. Comparison of analytical estimates $E^{(1)}$ [Eqs. (6)] and $E^{(2)}$ [Eqs. (7)] with numerical results calculated with the help of wave function (5) for several energy levels and given values of the Yukawa parameters B and C. Energy is expressed in units E_0.

B	C		$1s$	$2s$	$2p$	$3d$	$4f$	$5g$	$6h$	$7i$
1.5	10	$E^{(1)}$	-0.9583	-0.2449	-0.2500	-0.1111	-0.0625	-0.0400	-0.0278	-0.0204
		E	-0.9627	-0.2453	-0.2500	-0.1111	-0.0625	-0.0400	-0.0278	-0.0204
-1.5	0.2	$E^{(1)}$	-2.2397	-0.4453	-0.4308	-0.1456	-0.0689	-0.0410	-0.0279	-0.0204
		$E^{(2)}$	-2.7864	-0.5462	-0.5351	-0.1615	-0.0590	-0.0260	-0.0143	-0.0094
		E	-2.7864	-0.5474	-0.5363	-0.1675	-0.0716	-0.0412	-0.0279	-0.0204
-1.5	0.1	$E^{(1)}$	-2.3661	-0.5113	-0.5061	-0.1832	-0.0843	-0.0464	-0.0296	-0.0209
		$E^{(2)}$	-2.9187	-0.6383	-0.6348	-0.2267	-0.0964	-0.0451	-0.0231	-0.0131
		E	-2.9187	-0.6384	-0.6349	-0.2274	-0.0988	-0.0501	-0.0302	-0.0210
1	0.01	$E^{(2)}$	-0.2599	-0.0719	-0.0720	-0.0368	-0.0240	-0.0177	-0.0139	-0.0114
		E	-0.2599	-0.0719	-0.0720	-0.0368	-0.0241	-0.0178	-0.0141	-0.0116

$$E^{(2)}_{n,n-1}=\frac{B-2}{4n^2}\left[2+B-\frac{2B}{[nC/(2-B)+1]^{2n}}\right]. \tag{7b}$$

Expressions (7) are useful for $C \ll 1$ and $B<2$. If $C \to 0$ they go over into the hydrogenlike levels $E_n^{(2)} = -(2-B)^2/4n^2$ [cf. Eq. (4)]. The upper bounds given by Eqs. (6) and (7) are in general worse than those obtained with the use of the trial function (5) (see Table XII), although they provide accurate energy eigenvalues in the case when the potential is almost Coulombic, i.e., for very small or very large C, small $|B|$ or $B \ll -1$, and large n.

IV. CONCLUSIONS

In the present work the discrete energy eigenvalues for the superposition of the Coulomb and the Yukawa potentials have been calculated as functions of the strength B and the screening parameter C of the Yukawa potential. For $B=0$ the spectrum is given by $E_n^{\mathrm{H}}=-1/n^2$. The energy eigenvalues E_{nl} for the SCYP are shifted upwards or downwards with respect to the hydrogenlike levels E_n^{H} if $B>0$ or $B<0$, respectively. The absolute values of the deviations of E_{nl} from E_n^{H}, i.e., $|E_{nl}-E_n^{\mathrm{H}}|$, decrease with the increasing azimuthal quantum number l, which results in the corresponding ordering of the energy levels for a given n. This is due to the influence of the finite-range Yukawa potential, which decreases with increasing l. For certain values of B and C it yields the level crossing. For positive B and for $C \le C_0(B)$ the levels E_{2s}, E_{3s}, etc., lie above E_{3d}, E_{4f}, etc., respectively. On the contrary, for negative B and for C from the intervals $C_1(B) \le C \le C_2(B)$ the levels E_{4s}, E_{5s}, etc., are located below E_{3d}, E_{4f}, etc., respectively.

The energy eigenvalues considered as functions of B vary almost linearly if $|B| \ll 1$ [cf. Eqs. (6)] and are approximately quadratic functions of B if $B \ll -1$ [cf. Eq. (4)]. The dependence of E_{nl} on C shows two hydrogenlike limits for $C \to 0$ and $C \to \infty$. The difference between the spectra for the SCYP and for the purely Coulombic potential is largest for the intermediate values of the screening parameter $0.1 \lesssim C \lesssim 2$, i.e., for the screening length $10 \gtrsim D/a_0 \gtrsim 0.5$, provided that $B \gtrsim -10$. In this case the splittings of the energy levels with the same n and various l take also the largest values. If $B \to -\infty$ this interval shifts towards larger values of C.

The properties of the energy spectrum for the SCYP obtained in the present work have many analogies in atomic, solid-state, and quark physics. Property (i), giving the order of the energy levels E_{nl} with the same n, dependent on l and on the sign of the Yukawa potential, has an application to such systems as an exciton and a bound polaron in polar semiconductors and ionic crystals. These systems consist of two oppositely charged particles interacting with themselves through a polarizable medium. The energy levels of both the systems exhibit property (i),[5,7] although the total effective potential is even more complicated than the SCYP, being a linear combination of the Coulomb potential and an additional potential, which is a sum of two Yukawa potentials with different strengths and screening parameters, and an exponential potential. However, the net contribution of the additional potential is negative for the exciton[5,6] and positive for the bound polaron,[7] and one of the Yukawa potentials dominates at small distances.

Another system, having the energy levels ordered similarly to those for the SCYP with $B>0$, is the charmonium (the bound state of heavy charmed quark-antiquark pair). For each n the energy levels of charmonium increase with decreasing l.[12] This can be explained in the frames of the simple model,[13] assuming that the quark interact via the potential being the superposition of the attractive Coulomb potential and the positive linear potential.

ACKNOWLEDGMENTS

I would like to thank Dr. S. Bednarek for fruitful discussions. I am grateful to Professor B. Gerlach and Professor J. Treusch for kind hospitality during my stay at the University of Dortmund and for stimulating conversations. I wish also to thank Dr. G. Kasperidus for bringing to my attention Refs. 10—13. This work was supported in part by the Institute of Physics of the Polish Academy of Sciences.

---

[1] F. J. Rogers, H. C. Graboske, Jr., and D. J. Harwood, Phys. Rev. A **1**, 1577 (1970).

[2] K. M. Roussel and R. F. O'Connel, Phys. Rev. A **9**, 52 (1974).

[3] C. S. Lam and Y. P. Varshni, Phys. Rev. A **6**, 1391 (1972).

[4] C. S. Lai, Phys. Rev. A **26**, 2245 (1982).

[5] S. Bednarek, J. Adamowski, and M. Suffczyński, Solid State Commun. **21**, 1 (1977).

[6] J. Pollmann and H. Büttner, Phys. Rev. B **16**, 4480 (1977); H. Büttner and J. Pollmann, Physica (Utrecht) **117/118B**, 278 (1983).

[7] J. Adamowski, in *Proceedings of the XII Conference on Physics of Semiconducting Compounds, Jaszowiec, Poland, 1983* (Ossolineum, Wrocław, 1983), p. 139; and unpublished.

[8] P.-O. Löwdin, Phys. Rev. **139**, A357 (1965).

[9] G. W. F. Drake, Adv. At. Mol. Phys. **18**, 399 (1982).

[10] A. Martin, Phys. Lett. **67B**, 330 (1977).

[11] H. Grosse, Phys. Lett. **68B**, 343 (1977).

[12] M. Krammer and H. Krasemann, Acta Phys. Austr. Suppl. XXI, 259 (1979).

[13] E. Eichten, K. Gottfried, T. Kinoshita, J. Kogut, K. D. Lane, and T.-M. Yan, Phys. Rev. Lett. **34**, 369 (1975).